Amine, Amido, and Imido Complexes of Tantalum Supported by a Pyridine-Linked Bis(phenolate) Pincer Ligand. Ta-N p Bonding Influences Pincer Ligand Geometry.

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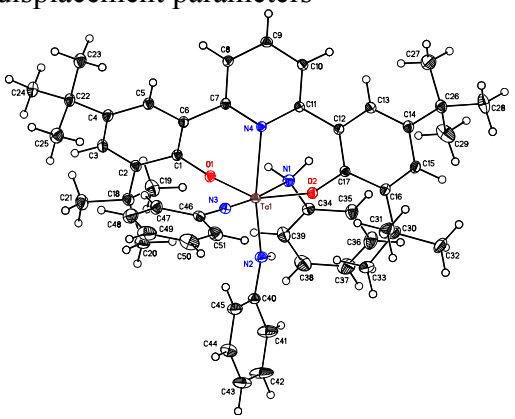
Supporting Information

Contents

Crystal Structure Analysis of:

Complex 1 (IAT03)

Contents



IAT03

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 680573. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 680573."

Table 1. Crystal data and structure refinement for IAT03 (CCDC 680573).

Empirical formula	$C_{51}H_{61}N_4O_2Ta \bullet 1½(C_6H_6)$
Formula weight	1060.15
Crystallization Solvent	Benzene
Crystal Habit	Fragment
Crystal size	0.22 x 0.18 x 0.15 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9678 reflections used in lattice determination	2.45 to 43.03°
Unit cell dimensions	a = 25.7250(8) Å b = 17.8546(5) Å β= 105.9790(10)° c = 23.6141(7) Å
Volume	10427.1(5) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	C2/c
Density (calculated)	1.351 Mg/m^3
F(000)	4376
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	2.07 to 43.26°
Completeness to θ = 43.26°	97.4 %
Index ranges	$-49 \le h \le 48$, $-32 \le k \le 33$, $-44 \le l \le 45$
Data collection scan type	ω scans; 16 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	233565
Independent reflections	38134 [R_{int}= 0.0821]
Absorption coefficient	2.154 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.7382 and 0.6486

Table 1 (cont.)

Structure solution and Refinement

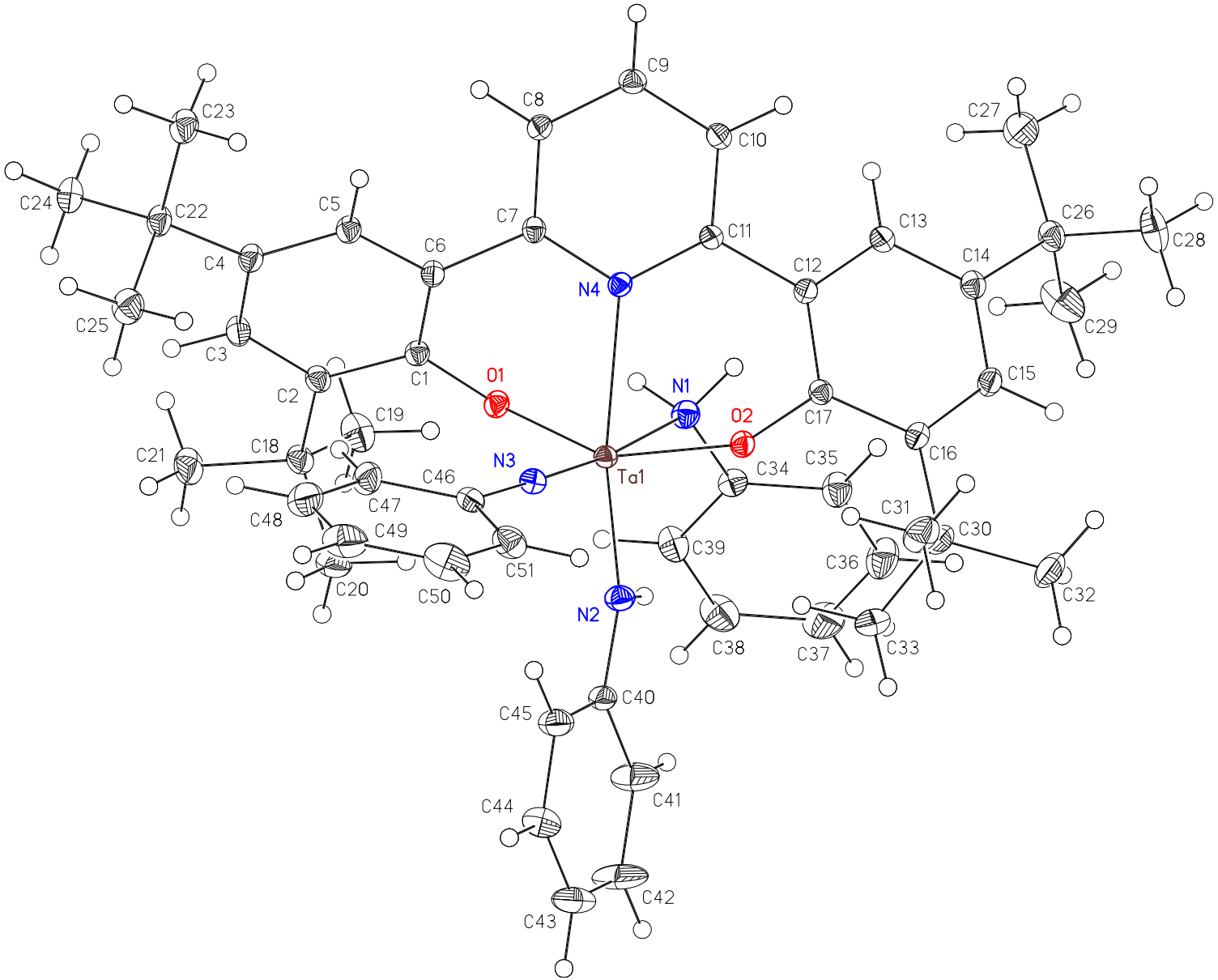
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	38134 / 0 / 617
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.117
Final R indices [$I>2\sigma(I)$, 25419 reflections]	R1 = 0.0299, *w*R2 = 0.0520
R indices (all data)	R1 = 0.0611, *w*R2 = 0.0557
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.009
Average shift/error	0.000
Largest diff. peak and hole	3.085 and -2.632 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C9
C8
C10
C23
C27
C24
C22
C5
C7
C11
C13
C26
C28
C4
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C14
N4
C25
C29
C3
C1
O1
N1
C15
C2
C19
C17
O2
C21
C18
N3
Ta1
C34
C35
C16
C46
C47
C31
C48
C49
C39
C30
C36
C51
C20
C50
C32
N2
C38
C37
C33
C40
C45
C41
C44
C42
C43

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT03 (CCDC 680573). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	1305(1)	10037(1)	1393(1)	10(1)
O(1)	1020(1)	10606(1)	1975(1)	13(1)
O(2)	1236(1)	9210(1)	806(1)	12(1)
N(1)	1076(1)	9102(1)	2062(1)	14(1)
N(2)	2063(1)	9811(1)	1897(1)	14(1)
N(3)	1436(1)	10802(1)	963(1)	13(1)
N(4)	377(1)	9973(1)	1003(1)	10(1)
C(1)	747(1)	11249(1)	1834(1)	11(1)
C(2)	886(1)	11880(1)	2210(1)	13(1)
C(3)	628(1)	12553(1)	2013(1)	14(1)
C(4)	236(1)	12634(1)	1467(1)	14(1)
C(5)	83(1)	11995(1)	1132(1)	13(1)
C(6)	320(1)	11294(1)	1312(1)	12(1)
C(7)	83(1)	10615(1)	982(1)	11(1)
C(8)	-467(1)	10632(1)	669(1)	13(1)
C(9)	-714(1)	10003(1)	372(1)	13(1)
C(10)	-420(1)	9350(1)	412(1)	13(1)
C(11)	123(1)	9340(1)	740(1)	11(1)
C(12)	412(1)	8616(1)	798(1)	11(1)
C(13)	134(1)	7958(1)	861(1)	13(1)
C(14)	380(1)	7262(1)	909(1)	13(1)
C(15)	901(1)	7235(1)	822(1)	14(1)
C(16)	1192(1)	7866(1)	750(1)	13(1)
C(17)	956(1)	8574(1)	786(1)	11(1)
C(18)	1319(1)	11824(1)	2807(1)	15(1)
C(19)	1173(1)	11197(1)	3181(1)	22(1)
C(20)	1876(1)	11671(1)	2709(1)	23(1)
C(21)	1356(1)	12546(1)	3164(1)	22(1)
C(22)	35(1)	13418(1)	1243(1)	15(1)
C(24)	-102(1)	13893(1)	1721(1)	19(1)
C(23)	-471(1)	13383(1)	716(1)	19(1)
C(25)	495(1)	13800(1)	1052(1)	21(1)
C(26)	118(1)	6550(1)	1067(1)	16(1)
C(27)	-452(1)	6692(1)	1123(1)	30(1)
C(28)	82(1)	5943(1)	602(1)	26(1)
C(29)	468(1)	6256(1)	1663(1)	30(1)
C(30)	1749(1)	7810(1)	630(1)	18(1)
C(32)	1914(1)	6996(1)	586(1)	28(1)
C(31)	1721(1)	8201(1)	44(1)	24(1)
C(33)	2193(1)	8182(1)	1126(1)	24(1)
C(34)	1443(1)	8610(1)	2466(1)	14(1)
C(35)	1480(1)	7864(1)	2323(1)	19(1)
C(36)	1849(1)	7396(1)	2703(1)	25(1)
C(37)	2184(1)	7677(1)	3227(1)	27(1)
C(38)	2144(1)	8421(1)	3369(1)	25(1)
C(39)	1773(1)	8894(1)	2991(1)	19(1)
C(40)	2600(1)	9999(1)	1928(1)	15(1)

C(41)	3024(1)	9629(1)	2336(1)	27(1)
C(42)	3560(1)	9799(1)	2368(1)	35(1)
C(43)	3686(1)	10331(1)	2002(1)	27(1)
C(44)	3269(1)	10698(1)	1599(1)	23(1)
C(45)	2732(1)	10533(1)	1562(1)	20(1)
C(46)	1535(1)	11428(1)	661(1)	13(1)
C(47)	1420(1)	12149(1)	825(1)	19(1)
C(48)	1533(1)	12772(1)	527(1)	26(1)
C(49)	1756(1)	12688(1)	58(1)	28(1)
C(50)	1868(1)	11982(1)	-111(1)	28(1)
C(51)	1763(1)	11352(1)	190(1)	20(1)
C(61)	2518(1)	210(1)	4402(1)	42(1)
C(62)	2770(1)	144(1)	3966(1)	39(1)
C(63)	3323(1)	-13(1)	4102(1)	34(1)
C(64)	3609(1)	-102(1)	4685(1)	35(1)
C(65)	3354(1)	-32(1)	5126(1)	38(1)
C(66)	2807(1)	123(1)	4986(1)	42(1)
C(71)	10000	9883(1)	2500	21(1)
C(72)	9679(1)	9489(1)	2022(1)	22(1)
C(73)	9675(1)	8714(1)	2025(1)	25(1)
C(74)	10000	8323(1)	2500	26(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT03 (CCDC 680573).

Ta(1)-N(4)	2.3112(8)	N(3)-Ta(1)-O(2)	99.52(4)
Ta(1)-O(2)	1.9999(9)	N(3)-Ta(1)-O(1)	99.46(4)
Ta(1)-O(1)	2.0013(9)	O(2)-Ta(1)-O(1)	150.56(3)
		N(3)-Ta(1)-N(2)	100.59(4)
Ta(1)-N(1)	2.4785(11)	O(2)-Ta(1)-N(2)	98.40(4)
Ta(1)-N(2)	2.0272(9)	O(1)-Ta(1)-N(2)	99.98(4)
Ta(1)-N(3)	1.7872(10)	N(3)-Ta(1)-N(4)	98.47(4)
		O(2)-Ta(1)-N(4)	78.60(3)
		O(1)-Ta(1)-N(4)	76.51(3)
		N(2)-Ta(1)-N(4)	160.94(4)
		N(3)-Ta(1)-N(1)	172.49(4)
		O(2)-Ta(1)-N(1)	87.29(4)
		O(1)-Ta(1)-N(1)	73.04(4)
		N(2)-Ta(1)-N(1)	81.39(4)
		N(4)-Ta(1)-N(1)	79.68(3)
N(1)-C(34)	1.4401(15)	C(34)-N(1)-Ta(1)	127.22(7)
N(2)-C(40)	1.4018(14)	C(40)-N(2)-Ta(1)	139.23(8)
N(3)-C(46)	1.3880(16)	C(46)-N(3)-Ta(1)	176.04(9)

Table 4. Bond lengths [Å] and angles [°] for IAT03 (CCDC 680573).

Ta(1)-N(3)	1.7872(10)	C(37)-C(38)	1.381(2)
Ta(1)-O(2)	1.9999(9)	C(38)-C(39)	1.3961(19)
Ta(1)-O(1)	2.0013(9)	C(40)-C(45)	1.3899(19)
Ta(1)-N(2)	2.0272(9)	C(40)-C(41)	1.4061(18)
Ta(1)-N(4)	2.3112(8)	C(41)-C(42)	1.394(2)
Ta(1)-N(1)	2.4785(11)	C(42)-C(43)	1.380(2)
O(1)-C(1)	1.3396(14)	C(43)-C(44)	1.388(2)
O(2)-C(17)	1.3387(14)	C(44)-C(45)	1.3913(18)
N(1)-C(34)	1.4401(15)	C(46)-C(51)	1.3991(18)
N(2)-C(40)	1.4018(14)	C(46)-C(47)	1.3994(18)
N(3)-C(46)	1.3880(16)	C(47)-C(48)	1.389(2)
N(4)-C(11)	1.3662(15)	C(48)-C(49)	1.388(2)
N(4)-C(7)	1.3672(15)	C(49)-C(50)	1.376(3)
C(1)-C(6)	1.4103(15)	C(50)-C(51)	1.395(2)
C(1)-C(2)	1.4166(16)	C(61)-C(62)	1.365(3)
C(2)-C(3)	1.3898(17)	C(61)-C(66)	1.383(3)
C(2)-C(18)	1.5403(16)	C(62)-C(63)	1.398(3)
C(3)-C(4)	1.4068(16)	C(63)-C(64)	1.380(3)
C(4)-C(5)	1.3843(17)	C(64)-C(65)	1.381(3)
C(4)-C(22)	1.5344(17)	C(65)-C(66)	1.383(3)
C(5)-C(6)	1.4056(16)	C(71)-C(72)#1	1.3903(18)
C(6)-C(7)	1.4788(16)	C(71)-C(72)	1.3904(18)
C(7)-C(8)	1.4046(16)	C(72)-C(73)	1.385(2)
C(8)-C(9)	1.3838(17)	C(73)-C(74)	1.387(2)
C(9)-C(10)	1.3784(17)	C(74)-C(73)#1	1.387(2)
C(10)-C(11)	1.3979(16)		
C(11)-C(12)	1.4793(16)	N(3)-Ta(1)-O(2)	99.52(4)
C(12)-C(13)	1.4049(16)	N(3)-Ta(1)-O(1)	99.46(4)
C(12)-C(17)	1.4072(15)	O(2)-Ta(1)-O(1)	150.56(3)
C(13)-C(14)	1.3836(17)	N(3)-Ta(1)-N(2)	100.59(4)
C(14)-C(15)	1.4117(17)	O(2)-Ta(1)-N(2)	98.40(4)
C(14)-C(26)	1.5330(17)	O(1)-Ta(1)-N(2)	99.98(4)
C(15)-C(16)	1.3902(17)	N(3)-Ta(1)-N(4)	98.47(4)
C(16)-C(17)	1.4148(16)	O(2)-Ta(1)-N(4)	78.60(3)
C(16)-C(30)	1.5379(17)	O(1)-Ta(1)-N(4)	76.51(3)
C(18)-C(21)	1.5297(18)	N(2)-Ta(1)-N(4)	160.94(4)
C(18)-C(19)	1.5347(19)	N(3)-Ta(1)-N(1)	172.49(4)
C(18)-C(20)	1.5391(18)	O(2)-Ta(1)-N(1)	87.29(4)
C(22)-C(24)	1.5300(18)	O(1)-Ta(1)-N(1)	73.04(4)
C(22)-C(23)	1.5352(17)	N(2)-Ta(1)-N(1)	81.39(4)
C(22)-C(25)	1.5360(19)	N(4)-Ta(1)-N(1)	79.68(3)
C(26)-C(28)	1.527(2)	C(1)-O(1)-Ta(1)	122.09(7)
C(26)-C(27)	1.5304(19)	C(17)-O(2)-Ta(1)	126.53(7)
C(26)-C(29)	1.5381(19)	C(34)-N(1)-Ta(1)	127.22(7)
C(30)-C(32)	1.526(2)	C(40)-N(2)-Ta(1)	139.23(8)
C(30)-C(31)	1.534(2)	C(46)-N(3)-Ta(1)	176.04(9)
C(30)-C(33)	1.544(2)	C(11)-N(4)-C(7)	119.09(9)
C(34)-C(35)	1.3839(19)	C(11)-N(4)-Ta(1)	122.35(7)
C(34)-C(39)	1.3919(17)	C(7)-N(4)-Ta(1)	118.20(7)
C(35)-C(36)	1.3921(19)	O(1)-C(1)-C(6)	119.63(10)
C(36)-C(37)	1.391(2)	O(1)-C(1)-C(2)	120.14(10)

C(6)-C(1)-C(2)	120.22(10)	C(28)-C(26)-C(27)	108.13(12)
C(3)-C(2)-C(1)	117.56(10)	C(28)-C(26)-C(14)	110.87(11)
C(3)-C(2)-C(18)	121.41(10)	C(27)-C(26)-C(14)	112.29(11)
C(1)-C(2)-C(18)	121.01(10)	C(28)-C(26)-C(29)	108.74(12)
C(2)-C(3)-C(4)	123.50(11)	C(27)-C(26)-C(29)	108.09(13)
C(5)-C(4)-C(3)	117.24(11)	C(14)-C(26)-C(29)	108.63(10)
C(5)-C(4)-C(22)	122.55(10)	C(32)-C(30)-C(31)	108.41(12)
C(3)-C(4)-C(22)	119.97(11)	C(32)-C(30)-C(16)	111.41(11)
C(4)-C(5)-C(6)	121.96(10)	C(31)-C(30)-C(16)	108.74(10)
C(5)-C(6)-C(1)	118.97(10)	C(32)-C(30)-C(33)	107.54(11)
C(5)-C(6)-C(7)	119.28(10)	C(31)-C(30)-C(33)	109.27(12)
C(1)-C(6)-C(7)	121.52(10)	C(16)-C(30)-C(33)	111.40(11)
N(4)-C(7)-C(8)	120.33(10)	C(35)-C(34)-C(39)	120.08(11)
N(4)-C(7)-C(6)	121.72(9)	C(35)-C(34)-N(1)	120.14(11)
C(8)-C(7)-C(6)	117.84(10)	C(39)-C(34)-N(1)	119.75(11)
C(9)-C(8)-C(7)	120.27(11)	C(34)-C(35)-C(36)	120.08(12)
C(10)-C(9)-C(8)	119.03(10)	C(37)-C(36)-C(35)	120.12(14)
C(9)-C(10)-C(11)	119.65(11)	C(38)-C(37)-C(36)	119.63(13)
N(4)-C(11)-C(10)	121.41(10)	C(37)-C(38)-C(39)	120.61(13)
N(4)-C(11)-C(12)	120.99(9)	C(34)-C(39)-C(38)	119.47(13)
C(10)-C(11)-C(12)	117.59(10)	C(45)-C(40)-N(2)	122.52(10)
C(13)-C(12)-C(17)	119.67(10)	C(45)-C(40)-C(41)	118.10(11)
C(13)-C(12)-C(11)	118.89(10)	N(2)-C(40)-C(41)	119.37(12)
C(17)-C(12)-C(11)	121.44(10)	C(42)-C(41)-C(40)	120.27(14)
C(14)-C(13)-C(12)	121.68(10)	C(43)-C(42)-C(41)	121.04(14)
C(13)-C(14)-C(15)	116.72(11)	C(42)-C(43)-C(44)	118.94(12)
C(13)-C(14)-C(26)	122.91(11)	C(43)-C(44)-C(45)	120.59(14)
C(15)-C(14)-C(26)	120.34(11)	C(40)-C(45)-C(44)	121.06(12)
C(16)-C(15)-C(14)	123.70(11)	N(3)-C(46)-C(51)	120.53(12)
C(15)-C(16)-C(17)	117.51(10)	N(3)-C(46)-C(47)	121.02(11)
C(15)-C(16)-C(30)	122.01(11)	C(51)-C(46)-C(47)	118.44(12)
C(17)-C(16)-C(30)	120.48(11)	C(48)-C(47)-C(46)	120.40(13)
O(2)-C(17)-C(12)	118.86(10)	C(49)-C(48)-C(47)	120.54(15)
O(2)-C(17)-C(16)	121.51(10)	C(50)-C(49)-C(48)	119.67(14)
C(12)-C(17)-C(16)	119.63(10)	C(49)-C(50)-C(51)	120.37(14)
C(21)-C(18)-C(19)	106.53(11)	C(50)-C(51)-C(46)	120.57(14)
C(21)-C(18)-C(20)	108.26(11)	C(62)-C(61)-C(66)	120.41(17)
C(19)-C(18)-C(20)	110.07(11)	C(61)-C(62)-C(63)	120.55(18)
C(21)-C(18)-C(2)	111.71(10)	C(64)-C(63)-C(62)	118.84(18)
C(19)-C(18)-C(2)	110.17(10)	C(63)-C(64)-C(65)	120.53(16)
C(20)-C(18)-C(2)	110.04(10)	C(64)-C(65)-C(66)	120.13(18)
C(24)-C(22)-C(4)	111.96(10)	C(61)-C(66)-C(65)	119.5(2)
C(24)-C(22)-C(23)	107.60(10)	C(72)#1-C(71)-C(72)	119.32(19)
C(4)-C(22)-C(23)	111.94(10)	C(73)-C(72)-C(71)	120.32(14)
C(24)-C(22)-C(25)	108.92(11)	C(72)-C(73)-C(74)	120.18(15)
C(4)-C(22)-C(25)	106.99(10)	C(73)-C(74)-C(73)#1	119.7(2)
C(23)-C(22)-C(25)	109.39(11)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+1/2

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT03 (CCDC 680573). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

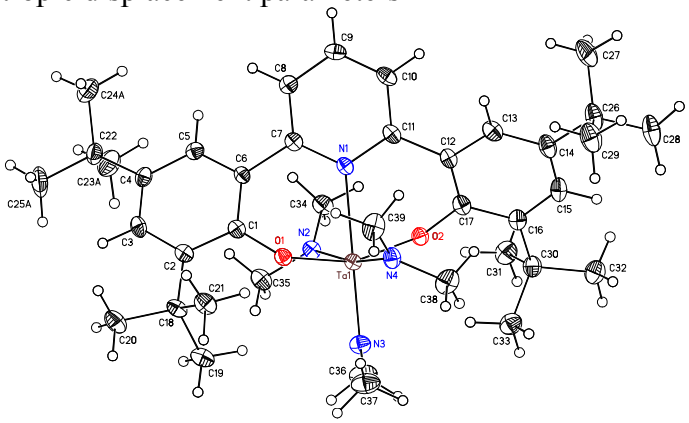
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	88(1)	96(1)	108(1)	6(1)	16(1)	0(1)
O(1)	133(4)	111(4)	121(3)	1(3)	11(3)	19(3)
O(2)	127(4)	101(4)	148(4)	-1(3)	49(3)	-2(3)
N(1)	145(4)	133(4)	142(4)	19(3)	35(3)	9(3)
N(2)	115(4)	149(5)	159(4)	24(3)	24(3)	6(3)
N(3)	115(4)	127(4)	135(4)	-3(3)	27(3)	-2(3)
N(4)	105(3)	103(4)	102(3)	4(3)	24(2)	10(3)
C(1)	121(4)	109(5)	112(4)	6(3)	27(3)	4(4)
C(2)	134(5)	125(5)	116(4)	-9(4)	18(4)	-7(4)
C(3)	172(5)	111(5)	140(4)	-10(4)	21(4)	0(4)
C(4)	152(5)	109(5)	140(4)	6(4)	34(4)	15(4)
C(5)	140(5)	113(5)	121(4)	3(4)	17(4)	9(4)
C(6)	129(4)	99(4)	112(4)	-4(3)	21(3)	5(4)
C(7)	129(4)	99(4)	101(4)	3(3)	27(3)	4(3)
C(8)	120(5)	114(5)	137(4)	0(4)	18(4)	15(4)
C(9)	110(4)	135(5)	134(3)	12(4)	15(3)	1(4)
C(10)	124(5)	117(5)	140(5)	-9(4)	20(4)	-11(4)
C(11)	106(4)	101(4)	122(4)	1(3)	30(3)	-4(3)
C(12)	115(4)	106(5)	119(4)	-5(3)	30(3)	7(3)
C(13)	123(5)	116(5)	140(5)	-4(4)	30(4)	-9(4)
C(14)	150(5)	114(5)	134(4)	4(4)	33(4)	-4(4)
C(15)	152(5)	107(5)	155(5)	-2(4)	33(4)	23(4)
C(16)	139(5)	111(5)	149(5)	1(4)	41(4)	18(4)
C(17)	117(4)	103(4)	111(4)	4(3)	27(3)	-3(3)
C(18)	156(5)	141(5)	130(4)	-15(4)	-1(4)	-3(4)
C(19)	288(7)	206(6)	123(5)	12(4)	9(4)	-26(5)
C(20)	149(5)	271(7)	233(6)	-46(5)	1(5)	-1(5)
C(21)	257(6)	189(6)	170(5)	-52(5)	-33(5)	18(5)
C(22)	181(5)	102(5)	149(5)	8(4)	26(4)	18(4)
C(24)	234(6)	130(5)	197(5)	-17(4)	64(5)	15(4)
C(23)	224(6)	142(5)	175(5)	19(4)	1(4)	36(4)
C(25)	237(6)	158(6)	229(6)	42(5)	80(5)	4(5)
C(26)	181(5)	115(5)	166(5)	17(4)	37(4)	-11(4)
C(27)	238(7)	173(6)	524(10)	45(6)	186(7)	-30(5)
C(28)	394(8)	144(6)	253(6)	-31(5)	113(6)	-80(5)
C(29)	338(8)	279(8)	225(6)	108(6)	-9(6)	-102(6)
C(30)	155(5)	137(5)	257(6)	6(4)	92(4)	32(4)
C(32)	225(6)	161(6)	515(10)	-13(6)	185(6)	52(5)
C(31)	243(6)	245(7)	273(7)	10(5)	161(5)	32(5)
C(33)	135(5)	231(7)	337(7)	-9(6)	29(5)	30(5)
C(34)	144(5)	143(5)	127(4)	32(4)	37(4)	12(4)
C(35)	234(6)	154(6)	164(5)	12(4)	27(4)	17(5)
C(36)	324(7)	165(6)	251(6)	51(5)	51(6)	67(5)
C(37)	250(7)	265(7)	255(7)	116(6)	-10(5)	52(6)
C(38)	256(7)	253(7)	176(5)	54(5)	-29(5)	-27(5)
C(39)	240(6)	163(6)	146(5)	9(4)	22(4)	-21(5)
C(40)	110(4)	167(5)	148(4)	-27(5)	9(3)	9(4)

C(41)	146(5)	379(9)	266(7)	127(6)	11(5)	27(6)
C(42)	114(5)	521(11)	363(8)	143(7)	-4(5)	37(6)
C(43)	121(5)	380(8)	281(7)	-18(6)	30(5)	-16(5)
C(44)	171(6)	268(7)	241(6)	6(5)	56(5)	-34(5)
C(45)	133(5)	211(6)	230(6)	33(5)	27(4)	5(4)
C(46)	115(4)	132(5)	134(4)	17(4)	17(4)	-19(4)
C(47)	203(6)	130(5)	257(6)	23(4)	99(5)	2(4)
C(48)	214(6)	158(6)	419(8)	94(6)	109(6)	13(5)
C(49)	207(6)	277(8)	357(8)	162(6)	76(6)	-25(5)
C(50)	273(7)	357(9)	221(6)	64(6)	105(5)	-78(6)
C(51)	199(6)	222(6)	196(5)	-17(5)	83(5)	-48(5)
C(61)	264(7)	241(8)	731(14)	28(8)	84(8)	-50(6)
C(62)	387(8)	194(8)	483(10)	-10(7)	-49(8)	-54(6)
C(63)	401(8)	197(7)	433(8)	-61(7)	104(7)	-24(7)
C(64)	296(7)	221(8)	495(9)	22(7)	66(7)	26(6)
C(65)	400(8)	280(8)	428(8)	75(8)	76(7)	-49(7)
C(66)	428(9)	293(9)	605(12)	40(8)	241(9)	-66(7)
C(71)	226(8)	187(9)	260(8)	0	137(6)	0
C(72)	223(6)	271(7)	201(6)	13(5)	116(5)	18(5)
C(73)	277(7)	270(7)	249(6)	-76(5)	154(5)	-35(5)
C(74)	340(11)	184(9)	345(11)	0	214(9)	0

Crystal Structure Analysis of:

Complex 2 (IAT09)

Contents



IAT09

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 693510. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 963510."

Table 1. Crystal data and structure refinement for IAT09 (CCDC 693510).

Empirical formula	$C_{39}H_{61}N_4O_2Ta$
Formula weight	798.87
Crystallization Solvent	Diethylether
Crystal Habit	Blade
Crystal size	0.22 x 0.11 x 0.03 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9936 reflections used in lattice determination	2.39 to 33.10°
Unit cell dimensions	a = 9.8149(5) Å b = 29.0840(14) Å β= 104.357(3)° c = 14.0826(6) Å
Volume	3894.4(3) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.363 Mg/m^3
F(000)	1648
θ range for data collection	1.65 to 33.20°
Completeness to θ = 33.20°	93.8 %
Index ranges	$-13 \le h \le 14$, $-39 \le k \le 43$, $-21 \le l \le 20$
Data collection scan type	ω scans; 7 settings
Reflections collected	53883
Independent reflections	13983 [R_{int}= 0.0450]
Absorption coefficient	2.858 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4353 and 0.3323

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	13983 / 0 / 449
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.426
Final R indices [$I>2\sigma(I)$, 10288 reflections]	R1 = 0.0350, *w*R2 = 0.0448
R indices (all data)	R1 = 0.0631, *w*R2 = 0.0471
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.666 and -1.582 e.Å^{-3}

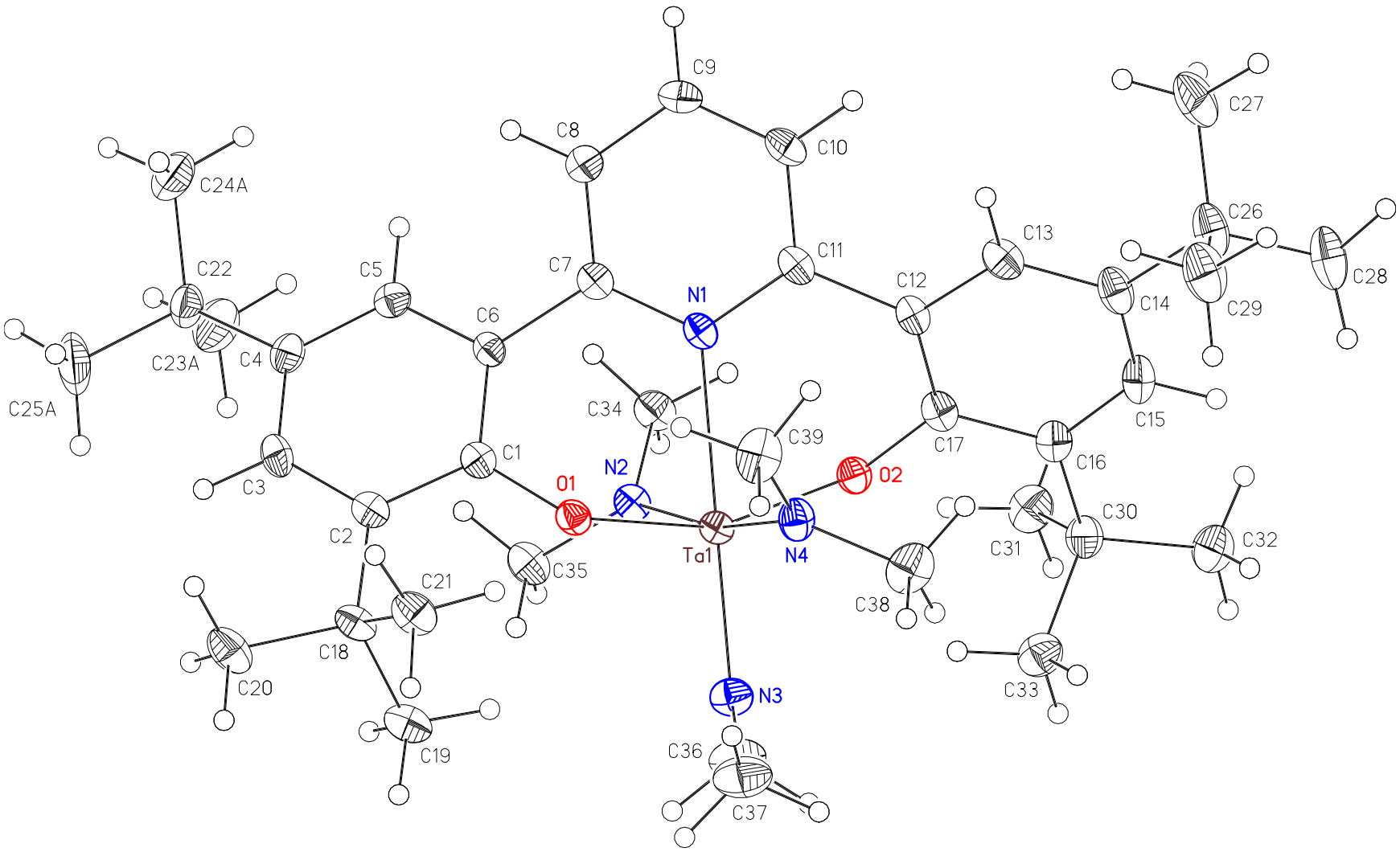
Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

One t-Bu group is disordered as shown in the third figure. The disorder is included in the model.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C22
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C29
C23A
C4
C25A
C34
C15
C39
C17
C1
N2
O2
C16
C3
O1
C30
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C20
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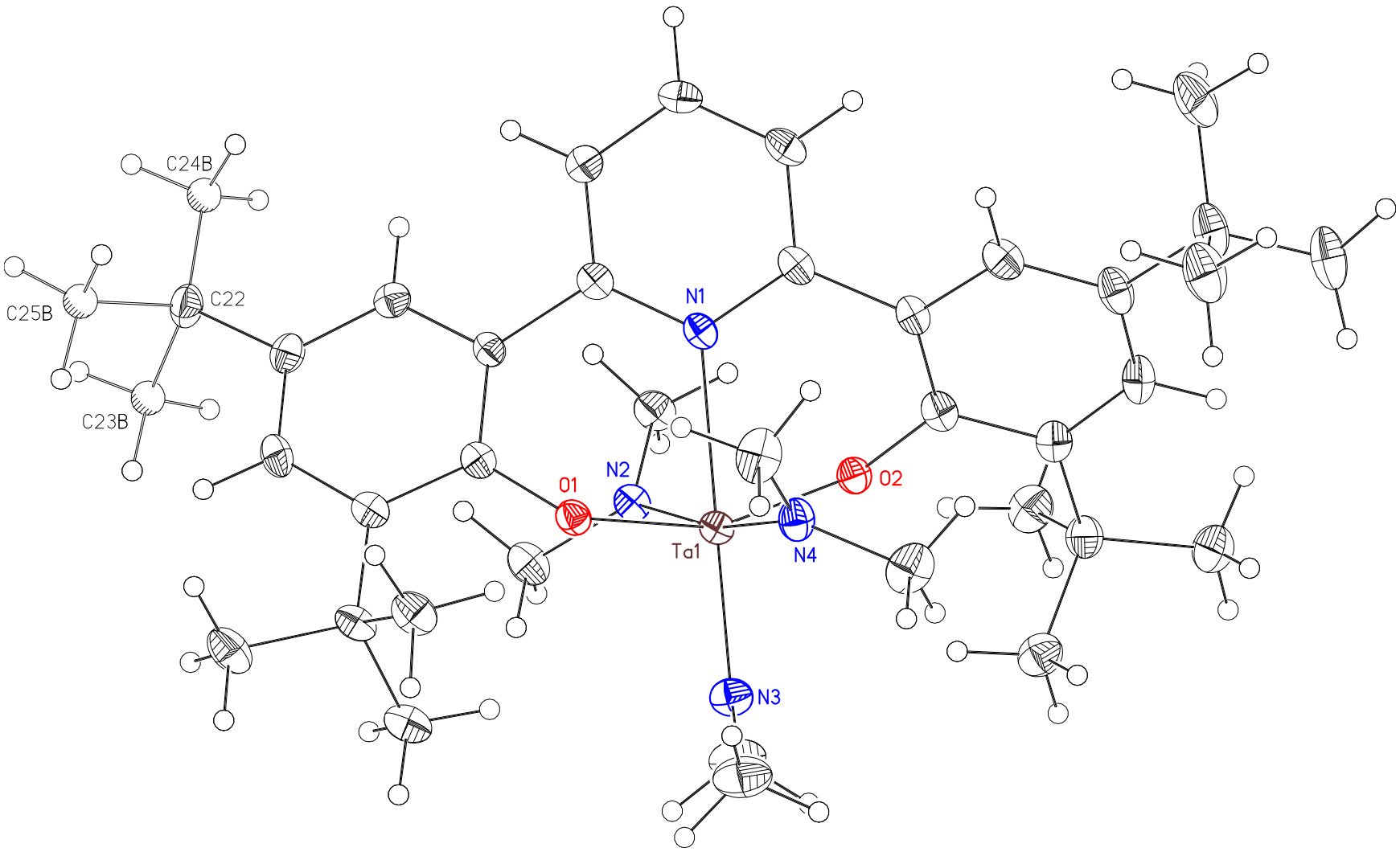
C19
C36
C37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C22
C25B
C23B
N1
N2
O1
O2
Ta1
N4
N3

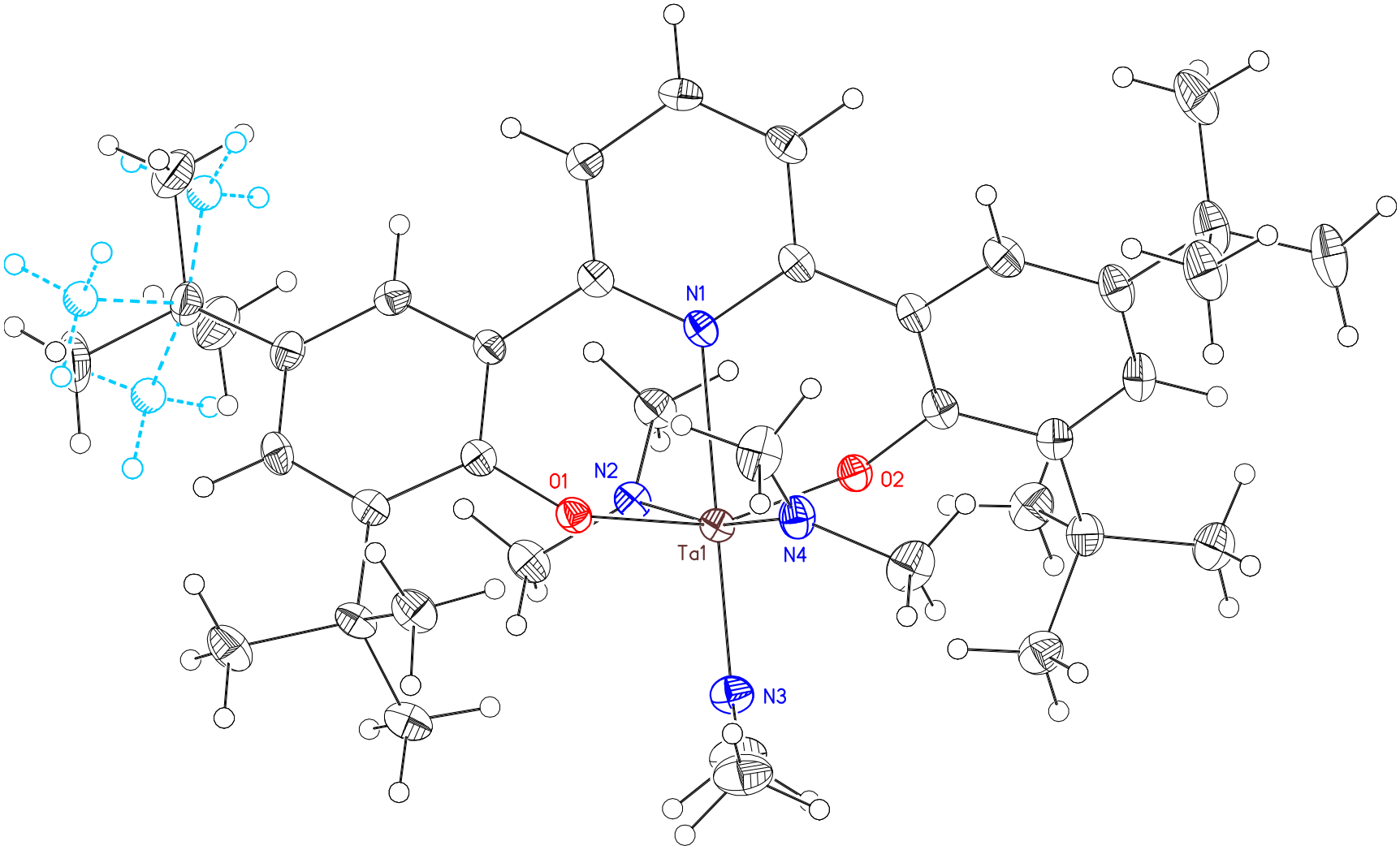

N1
O1
N2
Ta1
N4
O2
N3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT09 (CCDC 693510). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ta(1)	1345(1)	1155(1)	2702(1)	15(1)	1
O(1)	1189(2)	477(1)	2796(1)	17(1)	1
O(2)	1346(2)	1764(1)	2088(1)	17(1)	1
N(1)	894(2)	951(1)	1064(1)	16(1)	1
N(2)	3396(2)	1117(1)	2672(1)	18(1)	1
N(3)	1705(2)	1328(1)	4111(1)	21(1)	1
N(4)	-786(2)	1151(1)	2459(1)	21(1)	1
C(1)	1969(2)	164(1)	2467(2)	17(1)	1
C(2)	2507(2)	-219(1)	3039(2)	18(1)	1
C(3)	3510(2)	-485(1)	2743(2)	20(1)	1
C(4)	3959(2)	-388(1)	1890(2)	19(1)	1
C(5)	3260(2)	-48(1)	1286(2)	18(1)	1
C(6)	2239(2)	230(1)	1537(2)	15(1)	1
C(7)	1399(2)	548(1)	800(2)	16(1)	1
C(8)	1072(2)	411(1)	-175(2)	19(1)	1
C(9)	273(2)	691(1)	-886(2)	22(1)	1
C(10)	-197(2)	1101(1)	-621(2)	22(1)	1
C(11)	97(2)	1232(1)	365(2)	18(1)	1
C(12)	-434(2)	1682(1)	612(2)	18(1)	1
C(13)	-1656(2)	1866(1)	-14(2)	22(1)	1
C(14)	-2108(2)	2307(1)	87(2)	23(1)	1
C(15)	-1277(2)	2577(1)	830(2)	24(1)	1
C(16)	-75(2)	2417(1)	1498(2)	20(1)	1
C(17)	297(2)	1954(1)	1405(2)	19(1)	1
C(18)	2055(2)	-332(1)	3988(2)	21(1)	1
C(19)	2628(3)	29(1)	4782(2)	27(1)	1
C(20)	2596(3)	-803(1)	4398(2)	29(1)	1
C(21)	440(2)	-347(1)	3776(2)	25(1)	1
C(22)	5215(2)	-642(1)	1666(2)	23(1)	1
C(23A)	6447(3)	-294(1)	1834(2)	34(1)	0.888(5)
C(24A)	4870(4)	-799(1)	589(2)	36(1)	0.888(5)
C(25A)	5690(4)	-1055(1)	2310(3)	46(1)	0.888(5)
C(25B)	4880(30)	-1182(10)	1751(19)	36(6)	0.112(5)
C(23B)	6550(20)	-563(9)	2531(16)	29(6)	0.112(5)
C(24B)	5430(30)	-556(11)	726(18)	32(6)	0.112(5)
C(26)	-3486(2)	2486(1)	-584(2)	28(1)	1
C(27)	-3582(3)	2366(1)	-1661(2)	36(1)	1
C(28)	-3617(3)	3004(1)	-511(2)	38(1)	1
C(29)	-4722(2)	2258(1)	-267(2)	36(1)	1
C(30)	810(2)	2731(1)	2287(2)	22(1)	1
C(31)	2337(2)	2742(1)	2174(2)	28(1)	1
C(32)	271(3)	3224(1)	2202(2)	32(1)	1
C(33)	815(3)	2563(1)	3329(2)	27(1)	1
C(34)	4013(2)	1300(1)	1896(2)	23(1)	1
C(35)	4436(2)	842(1)	3352(2)	23(1)	1
C(36)	2921(3)	1581(1)	4660(2)	34(1)	1
C(37)	746(3)	1237(1)	4731(2)	36(1)	1
C(38)	-1601(2)	1538(1)	2691(2)	30(1)	1

C(39)	-1734(2)	800(1)	1941(2)	31(1)	1

Table 3. Selected bond lengths [Å] and angles [°] for IAT09 (CCDC 693510).

Ta(1)-O(2)	1.9721(16)	O(2)-Ta(1)-O(1)	158.51(6)
Ta(1)-O(1)	1.9848(16)	O(2)-Ta(1)-N(3)	100.93(7)
Ta(1)-N(3)	1.9914(18)	O(1)-Ta(1)-N(3)	100.55(7)
Ta(1)-N(2)	2.0270(16)	O(2)-Ta(1)-N(2)	86.07(7)
Ta(1)-N(4)	2.0336(17)	O(1)-Ta(1)-N(2)	92.31(7)
Ta(1)-N(1)	2.3156(17)	N(3)-Ta(1)-N(2)	95.91(7)
		O(2)-Ta(1)-N(4)	92.49(7)
		O(1)-Ta(1)-N(4)	84.98(8)
		N(3)-Ta(1)-N(4)	95.21(7)
		N(2)-Ta(1)-N(4)	168.86(7)
		O(2)-Ta(1)-N(1)	79.26(6)
		O(1)-Ta(1)-N(1)	79.25(6)
		N(3)-Ta(1)-N(1)	179.22(7)
		N(2)-Ta(1)-N(1)	84.85(6)
		N(4)-Ta(1)-N(1)	84.02(6)

Table 4. Bond lengths [Å] and angles [°] for IAT09 (CCDC 693510).

Ta(1)-O(2)	1.9721(16)	C(30)-C(33)	1.546(3)
Ta(1)-O(1)	1.9848(16)	C(30)-C(31)	1.547(3)
Ta(1)-N(3)	1.9914(18)		
Ta(1)-N(2)	2.0270(16)	O(2)-Ta(1)-O(1)	158.51(6)
Ta(1)-N(4)	2.0336(17)	O(2)-Ta(1)-N(3)	100.93(7)
Ta(1)-N(1)	2.3156(17)	O(1)-Ta(1)-N(3)	100.55(7)
O(1)-C(1)	1.343(3)	O(2)-Ta(1)-N(2)	86.07(7)
O(2)-C(17)	1.342(3)	O(1)-Ta(1)-N(2)	92.31(7)
N(1)-C(7)	1.361(3)	N(3)-Ta(1)-N(2)	95.91(7)
N(1)-C(11)	1.366(3)	O(2)-Ta(1)-N(4)	92.49(7)
N(2)-C(35)	1.454(3)	O(1)-Ta(1)-N(4)	84.98(8)
N(2)-C(34)	1.475(3)	N(3)-Ta(1)-N(4)	95.21(7)
N(3)-C(36)	1.450(3)	N(2)-Ta(1)-N(4)	168.86(7)
N(3)-C(37)	1.458(3)	O(2)-Ta(1)-N(1)	79.26(6)
N(4)-C(39)	1.451(3)	O(1)-Ta(1)-N(1)	79.25(6)
N(4)-C(38)	1.463(3)	N(3)-Ta(1)-N(1)	179.22(7)
C(1)-C(2)	1.398(3)	N(2)-Ta(1)-N(1)	84.85(6)
C(1)-C(6)	1.413(3)	N(4)-Ta(1)-N(1)	84.02(6)
C(2)-C(3)	1.396(3)	C(1)-O(1)-Ta(1)	126.16(13)
C(2)-C(18)	1.545(3)	C(17)-O(2)-Ta(1)	126.91(14)
C(3)-C(4)	1.407(3)	C(7)-N(1)-C(11)	119.99(18)
C(4)-C(5)	1.373(3)	C(7)-N(1)-Ta(1)	120.01(14)
C(4)-C(22)	1.536(3)	C(11)-N(1)-Ta(1)	119.98(15)
C(5)-C(6)	1.399(3)	C(35)-N(2)-C(34)	109.66(16)
C(6)-C(7)	1.478(3)	C(35)-N(2)-Ta(1)	123.71(13)
C(7)-C(8)	1.388(3)	C(34)-N(2)-Ta(1)	126.07(14)
C(8)-C(9)	1.375(3)	C(36)-N(3)-C(37)	109.94(18)
C(9)-C(10)	1.365(3)	C(36)-N(3)-Ta(1)	125.38(14)
C(10)-C(11)	1.398(3)	C(37)-N(3)-Ta(1)	124.63(15)
C(11)-C(12)	1.483(3)	C(39)-N(4)-C(38)	109.57(18)
C(12)-C(17)	1.410(3)	C(39)-N(4)-Ta(1)	126.43(16)
C(12)-C(13)	1.407(3)	C(38)-N(4)-Ta(1)	123.65(17)
C(13)-C(14)	1.376(3)	O(1)-C(1)-C(2)	120.42(18)
C(14)-C(15)	1.397(3)	O(1)-C(1)-C(6)	118.8(2)
C(14)-C(26)	1.536(3)	C(2)-C(1)-C(6)	120.8(2)
C(15)-C(16)	1.394(3)	C(3)-C(2)-C(1)	117.63(19)
C(16)-C(17)	1.409(3)	C(3)-C(2)-C(18)	121.0(2)
C(16)-C(30)	1.532(3)	C(1)-C(2)-C(18)	121.3(2)
C(18)-C(20)	1.529(4)	C(4)-C(3)-C(2)	122.5(2)
C(18)-C(19)	1.536(3)	C(5)-C(4)-C(3)	117.4(2)
C(18)-C(21)	1.539(3)	C(5)-C(4)-C(22)	121.5(2)
C(22)-C(24B)	1.41(2)	C(3)-C(4)-C(22)	121.1(2)
C(22)-C(25A)	1.506(4)	C(4)-C(5)-C(6)	122.6(2)
C(22)-C(24A)	1.538(4)	C(5)-C(6)-C(1)	117.8(2)
C(22)-C(23A)	1.551(4)	C(5)-C(6)-C(7)	119.58(18)
C(22)-C(23B)	1.57(2)	C(1)-C(6)-C(7)	122.37(19)
C(22)-C(25B)	1.61(3)	N(1)-C(7)-C(8)	120.4(2)
C(26)-C(28)	1.517(4)	N(1)-C(7)-C(6)	121.62(19)
C(26)-C(27)	1.538(3)	C(8)-C(7)-C(6)	117.9(2)
C(26)-C(29)	1.543(3)	C(9)-C(8)-C(7)	120.1(2)
C(30)-C(32)	1.521(4)	C(10)-C(9)-C(8)	119.2(2)

C(9)-C(10)-C(11)	120.6(2)	C(24A)-C(22)-C(4)	110.7(2)
N(1)-C(11)-C(10)	119.6(2)	C(24B)-C(22)-C(23A)	74.6(12)
N(1)-C(11)-C(12)	121.99(19)	C(25A)-C(22)-C(23A)	108.4(2)
C(10)-C(11)-C(12)	118.3(2)	C(24A)-C(22)-C(23A)	108.5(2)
C(17)-C(12)-C(13)	118.0(2)	C(4)-C(22)-C(23A)	106.7(2)
C(17)-C(12)-C(11)	122.8(2)	C(24B)-C(22)-C(23B)	114.2(13)
C(13)-C(12)-C(11)	118.9(2)	C(25A)-C(22)-C(23B)	64.9(10)
C(14)-C(13)-C(12)	122.4(2)	C(24A)-C(22)-C(23B)	138.2(8)
C(13)-C(14)-C(15)	117.2(2)	C(4)-C(22)-C(23B)	109.2(8)
C(13)-C(14)-C(26)	120.6(2)	C(23A)-C(22)-C(23B)	46.8(9)
C(15)-C(14)-C(26)	122.1(2)	C(24B)-C(22)-C(25B)	108.9(15)
C(16)-C(15)-C(14)	123.8(2)	C(25A)-C(22)-C(25B)	38.6(9)
C(15)-C(16)-C(17)	116.9(2)	C(24A)-C(22)-C(25B)	77.7(9)
C(15)-C(16)-C(30)	121.5(2)	C(4)-C(22)-C(25B)	105.4(9)
C(17)-C(16)-C(30)	121.6(2)	C(23A)-C(22)-C(25B)	142.2(10)
O(2)-C(17)-C(16)	119.8(2)	C(23B)-C(22)-C(25B)	103.3(13)
O(2)-C(17)-C(12)	119.1(2)	C(28)-C(26)-C(27)	107.9(2)
C(16)-C(17)-C(12)	121.1(2)	C(28)-C(26)-C(14)	111.8(2)
C(20)-C(18)-C(2)	111.8(2)	C(27)-C(26)-C(14)	111.0(2)
C(20)-C(18)-C(19)	107.98(19)	C(28)-C(26)-C(29)	108.8(2)
C(2)-C(18)-C(19)	110.55(19)	C(27)-C(26)-C(29)	109.1(2)
C(20)-C(18)-C(21)	107.0(2)	C(14)-C(26)-C(29)	108.2(2)
C(2)-C(18)-C(21)	109.93(18)	C(32)-C(30)-C(16)	112.4(2)
C(19)-C(18)-C(21)	109.5(2)	C(32)-C(30)-C(33)	107.0(2)
C(24B)-C(22)-C(25A)	127.6(12)	C(16)-C(30)-C(33)	111.6(2)
C(24B)-C(22)-C(24A)	34.7(12)	C(32)-C(30)-C(31)	107.4(2)
C(25A)-C(22)-C(24A)	108.6(3)	C(16)-C(30)-C(31)	109.10(19)
C(24B)-C(22)-C(4)	114.9(11)	C(33)-C(30)-C(31)	109.22(19)
C(25A)-C(22)-C(4)	113.8(2)		

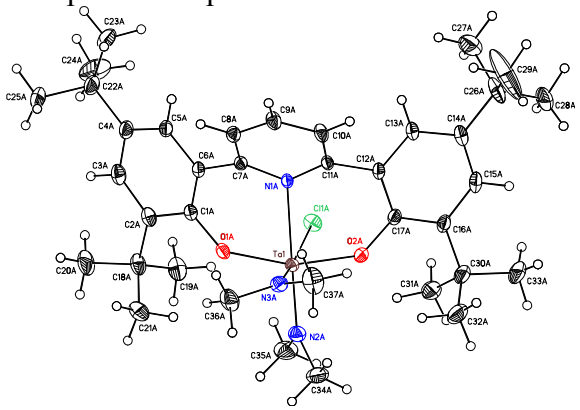
Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT09 (CCDC 693510). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	139(1)	170(1)	152(1)	9(1)	38(1)	-13(1)
O(1)	166(8)	193(10)	171(7)	29(7)	59(6)	10(7)
O(2)	152(8)	181(10)	187(7)	8(7)	36(6)	6(7)
N(1)	134(9)	166(12)	171(9)	35(8)	35(7)	-12(8)
N(2)	152(8)	188(12)	181(8)	14(9)	35(7)	-13(9)
N(3)	224(10)	215(13)	205(9)	5(8)	92(8)	-60(9)
N(4)	162(8)	209(12)	261(9)	25(10)	69(7)	19(10)
C(1)	125(10)	180(14)	182(10)	6(10)	18(8)	-21(10)
C(2)	162(11)	187(14)	176(10)	12(10)	28(9)	-35(10)
C(3)	199(12)	141(14)	247(12)	46(10)	30(10)	-5(10)
C(4)	201(11)	133(14)	236(11)	-27(10)	52(10)	-27(10)
C(5)	191(11)	159(14)	184(11)	-16(10)	55(9)	-34(10)
C(6)	154(10)	125(13)	162(10)	11(9)	13(9)	-28(9)
C(7)	117(10)	175(14)	187(10)	18(10)	44(9)	-36(9)
C(8)	191(11)	182(15)	200(11)	-5(10)	61(9)	-19(10)
C(9)	235(12)	264(17)	145(10)	-10(10)	30(9)	-30(11)
C(10)	186(10)	278(17)	178(10)	43(11)	-8(8)	5(11)
C(11)	146(10)	194(16)	190(10)	43(10)	21(8)	-18(10)
C(12)	154(11)	175(15)	204(11)	38(10)	30(9)	-3(10)
C(13)	176(11)	248(16)	225(11)	31(11)	18(9)	-27(11)
C(14)	160(11)	226(16)	301(12)	84(11)	56(10)	18(11)
C(15)	221(12)	166(15)	337(13)	40(11)	88(11)	28(11)
C(16)	178(11)	187(15)	243(11)	18(10)	66(10)	-4(10)
C(17)	151(11)	205(15)	226(11)	51(10)	74(9)	-8(10)
C(18)	209(12)	245(16)	169(10)	48(10)	36(9)	-19(11)
C(19)	295(13)	324(18)	194(11)	46(11)	52(10)	-22(12)
C(20)	280(14)	311(18)	272(13)	121(12)	71(11)	0(12)
C(21)	230(12)	287(17)	258(12)	72(11)	92(10)	-41(11)
C(22)	225(12)	194(15)	282(12)	18(11)	101(10)	59(11)
C(23A)	249(16)	370(20)	442(19)	-55(16)	126(14)	42(14)
C(24A)	390(19)	310(20)	368(18)	-88(16)	107(15)	87(17)
C(25A)	570(20)	340(30)	560(20)	204(18)	280(20)	281(19)
C(26)	174(12)	249(17)	403(15)	99(12)	41(11)	40(11)
C(27)	234(13)	430(20)	381(15)	132(14)	-15(12)	100(13)
C(28)	269(14)	299(19)	528(17)	122(15)	40(13)	103(13)
C(29)	184(12)	390(20)	482(16)	102(15)	47(12)	64(12)
C(30)	224(12)	187(15)	260(12)	9(11)	60(10)	-9(11)
C(31)	286(14)	213(16)	340(14)	-18(12)	97(12)	-70(12)
C(32)	391(16)	220(17)	335(14)	-21(12)	78(12)	7(13)
C(33)	289(14)	247(17)	284(13)	-31(12)	91(11)	-40(12)
C(34)	186(11)	279(17)	222(11)	37(10)	69(10)	2(10)
C(35)	164(11)	260(16)	241(12)	40(11)	10(10)	-31(11)
C(36)	376(16)	400(20)	243(13)	-71(13)	97(12)	-88(14)
C(37)	411(15)	460(20)	267(12)	-15(13)	185(12)	-69(14)
C(38)	226(13)	324(18)	398(14)	-7(13)	195(12)	-32(12)
C(39)	190(12)	282(18)	447(16)	-27(13)	87(12)	-43(12)

Crystal Structure Analysis of:

Complex 3 (IAT10)

Contents



IAT10

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 693797. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 693797."

Table 1. Crystal data and structure refinement for IAT10 (CCDC 693797).

Empirical formula	$C_{37}H_{55}N_3O_2ClTa \bullet 0.75(C_4H_{10}O)$
Formula weight	845.83
Crystallization Solvent	Diethylether
Crystal Habit	Block
Crystal size	0.29 x 0.28 x 0.23 mm^3
Crystal color	Pale yellow

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9746 reflections used in lattice determination	2.63 to 46.81°
Unit cell dimensions	a = 14.7164(6) Å b = 18.3370(7) Å β= 101.802(2)° c = 31.2188(13) Å
Volume	8246.4(6) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.363 Mg/m^3
F(000)	3484
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.68 to 47.98°
Completeness to θ = 47.98°	96.0 %
Index ranges	$-30 \le h \le 29$, $-38 \le k \le 37$, $-64 \le l \le 64$
Data collection scan type	ω scans; 25 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	492193
Independent reflections	75746 [R_{int}= 0.0554]
Absorption coefficient	2.767 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4493 and 0.3540

Table 1 (cont.)

Structure solution and Refinement

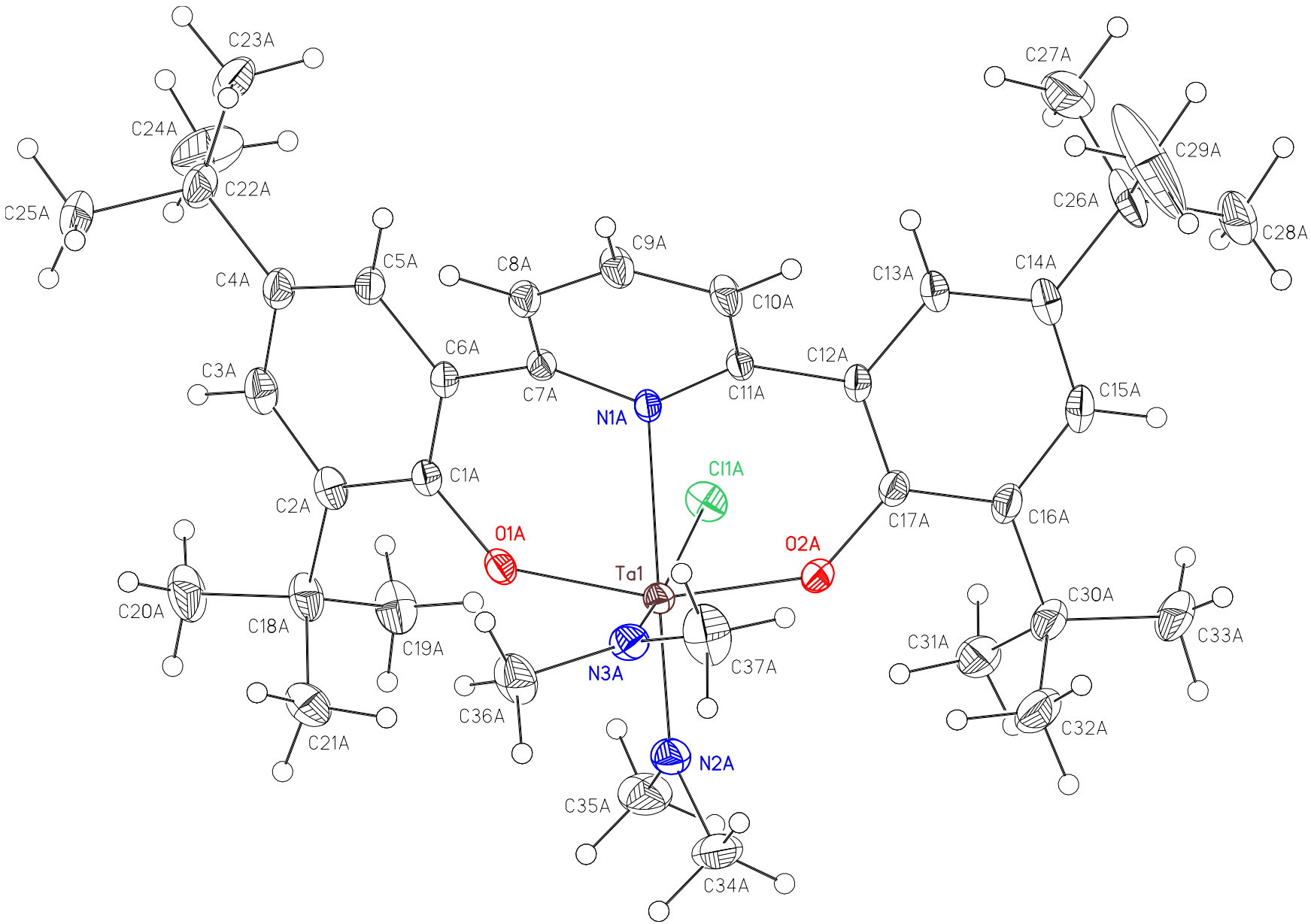
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	75746 / 0 / 905
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.760
Final R indices [$I>2\sigma(I)$, 50883 reflections]	R1 = 0.0731, *w*R2 = 0.1059
R indices (all data)	R1 = 0.1097, *w*R2 = 0.1074
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.004
Average shift/error	0.000
Largest diff. peak and hole	10.132 and -8.855 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C6A
C3A
C7A
N1A
C11A
C12A
C15A
C1A
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C2A
C17A
C16A
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O2A
Ta1
C20A
C18A
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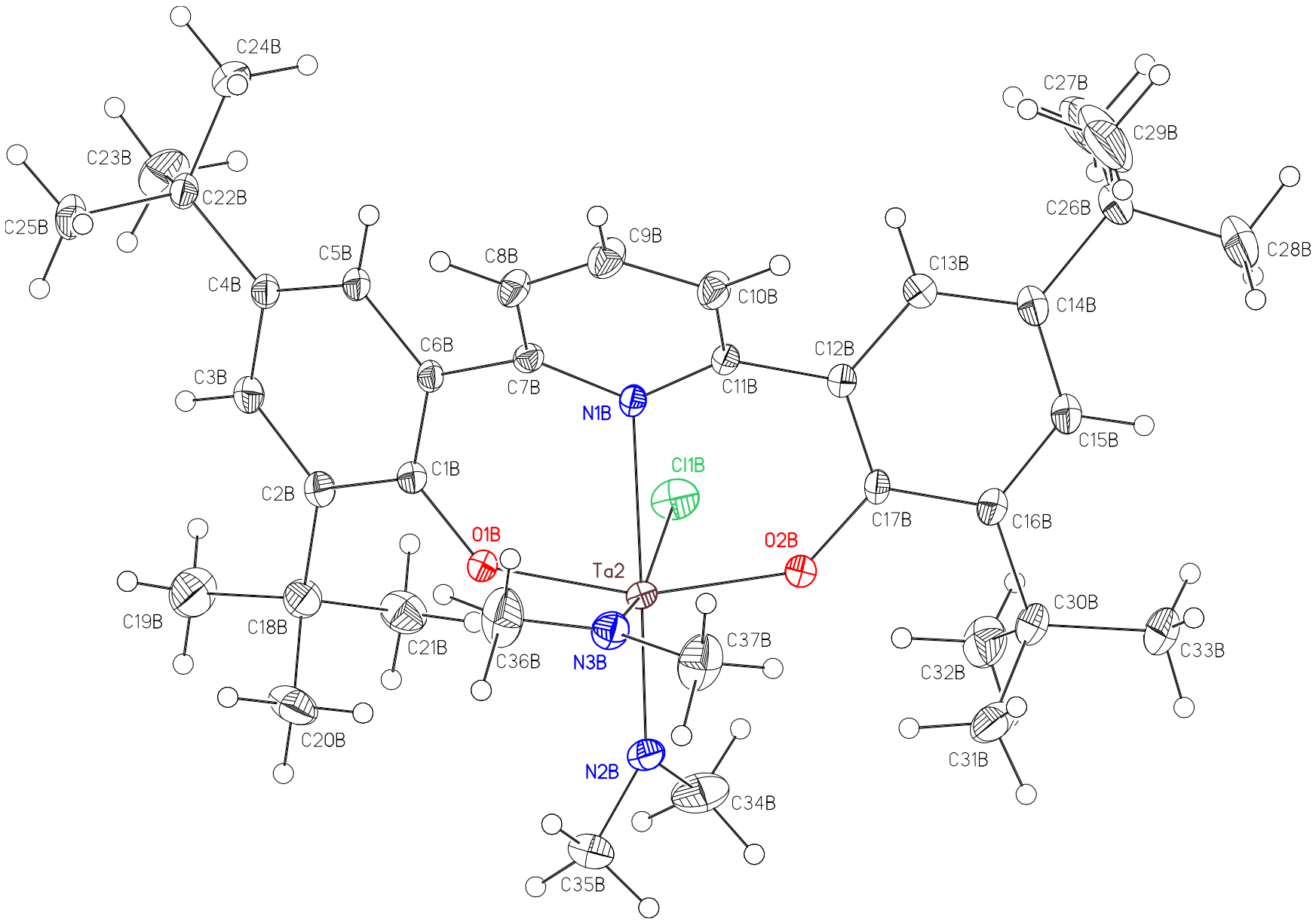
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C1B
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Cl1B
C17B
C16B
O1B
O2B
Ta2
C19B
C18B
C21B
C36B
N3B
C37B
C30B
C33B
C32B
C20B
C31B
N2B
C34B
C35B

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT10 (CCDC 693797). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	6285(1)	7674(1)	2306(1)	15(1)
Cl(1A)	4780(1)	7080(1)	2305(1)	21(1)
O(1A)	6501(1)	7630(1)	2936(1)	17(1)
O(2A)	5755(1)	7931(1)	1711(1)	18(1)
N(1A)	5468(1)	8751(1)	2438(1)	13(1)
N(2A)	6943(2)	6783(1)	2188(1)	23(1)
N(3A)	7327(1)	8353(1)	2289(1)	20(1)
C(1A)	6178(2)	7907(1)	3277(1)	16(1)
C(2A)	6265(2)	7497(1)	3669(1)	20(1)
C(3A)	5884(2)	7814(1)	4000(1)	23(1)
C(4A)	5460(2)	8500(1)	3970(1)	21(1)
C(5A)	5438(2)	8886(1)	3590(1)	18(1)
C(6A)	5799(2)	8600(1)	3240(1)	15(1)
C(7A)	5705(2)	9057(1)	2843(1)	14(1)
C(8A)	5782(2)	9813(1)	2893(1)	18(1)
C(9A)	5553(2)	10264(1)	2533(1)	22(1)
C(10A)	5188(2)	9952(1)	2131(1)	20(1)
C(11A)	5139(2)	9195(1)	2090(1)	14(1)
C(12A)	4661(2)	8882(1)	1666(1)	16(1)
C(13A)	3860(2)	9232(1)	1442(1)	18(1)
C(14A)	3365(2)	8970(1)	1044(1)	21(1)
C(15A)	3710(2)	8348(1)	873(1)	23(1)
C(16A)	4506(2)	7977(1)	1081(1)	20(1)
C(17A)	4973(2)	8253(1)	1486(1)	17(1)
C(18A)	6717(2)	6745(1)	3726(1)	24(1)
C(19A)	6065(2)	6198(1)	3444(1)	30(1)
C(20A)	6875(2)	6483(2)	4204(1)	35(1)
C(21A)	7678(2)	6752(2)	3598(1)	30(1)
C(22A)	5034(2)	8780(2)	4345(1)	27(1)
C(23A)	4576(2)	9532(2)	4251(1)	31(1)
C(24A)	4275(3)	8251(2)	4418(1)	49(1)
C(25A)	5785(3)	8863(3)	4761(1)	49(1)
C(26A)	2477(2)	9362(2)	811(1)	34(1)
C(27A)	1799(3)	9415(2)	1146(2)	52(1)
C(28A)	1942(2)	8937(2)	431(1)	40(1)
C(29A)	2695(4)	10121(3)	688(2)	101(3)
C(30A)	4866(2)	7303(2)	872(1)	29(1)
C(31A)	4892(2)	6636(2)	1171(1)	33(1)
C(32A)	5848(2)	7471(2)	793(1)	40(1)
C(33A)	4250(3)	7115(2)	430(1)	42(1)
C(34A)	7636(2)	6782(2)	1909(1)	32(1)
C(35A)	6777(2)	6051(1)	2327(1)	34(1)
C(36A)	8104(2)	8435(2)	2661(1)	31(1)
C(37A)	7418(2)	8875(2)	1947(1)	38(1)

Ta(2)	3444(1)	2681(1)	2235(1)	14(1)
Cl(1B)	4965(1)	2064(1)	2376(1)	24(1)
O(1B)	3667(1)	2893(1)	1662(1)	16(1)
O(2B)	3565(1)	2672(1)	2858(1)	18(1)
N(1B)	4417(1)	3736(1)	2408(1)	13(1)
N(2B)	2655(2)	1808(1)	2082(1)	22(1)
N(3B)	2429(1)	3406(1)	2150(1)	20(1)
C(1B)	4299(2)	3226(1)	1474(1)	16(1)
C(2B)	4534(2)	2933(1)	1093(1)	18(1)
C(3B)	5177(2)	3322(1)	912(1)	19(1)
C(4B)	5602(2)	3963(1)	1091(1)	16(1)
C(5B)	5346(2)	4232(1)	1464(1)	15(1)
C(6B)	4697(2)	3874(1)	1660(1)	14(1)
C(7B)	4508(1)	4186(1)	2071(1)	13(1)
C(8B)	4510(2)	4943(1)	2120(1)	18(1)
C(9B)	4453(2)	5247(1)	2518(1)	22(1)
C(10B)	4476(2)	4785(1)	2871(1)	21(1)
C(11B)	4479(2)	4034(1)	2812(1)	15(1)
C(12B)	4611(2)	3566(1)	3207(1)	17(1)
C(13B)	5230(2)	3802(1)	3581(1)	22(1)
C(14B)	5348(2)	3421(1)	3972(1)	23(1)
C(15B)	4819(2)	2796(1)	3982(1)	22(1)
C(16B)	4201(2)	2522(1)	3618(1)	19(1)
C(17B)	4127(2)	2914(1)	3223(1)	16(1)
C(18B)	4136(2)	2199(1)	899(1)	24(1)
C(19B)	4450(3)	2026(2)	470(1)	41(1)
C(20B)	3066(2)	2202(1)	796(1)	30(1)
C(21B)	4494(2)	1588(1)	1228(1)	27(1)
C(22B)	6312(2)	4352(1)	875(1)	18(1)
C(23B)	7017(2)	3806(2)	766(1)	33(1)
C(24B)	6851(2)	4936(2)	1174(1)	30(1)
C(25B)	5801(2)	4714(2)	453(1)	27(1)
C(26B)	6058(2)	3681(2)	4374(1)	30(1)
C(27B)	7029(3)	3495(4)	4311(2)	80(2)
C(28B)	5921(3)	3315(2)	4794(1)	44(1)
C(29B)	5956(5)	4502(2)	4441(2)	81(2)
C(30B)	3646(2)	1820(1)	3641(1)	26(1)
C(31B)	2610(2)	1906(2)	3433(1)	34(1)
C(32B)	4077(2)	1214(1)	3402(1)	34(1)
C(33B)	3703(3)	1575(2)	4112(1)	36(1)
C(34B)	2932(2)	1060(1)	2205(1)	36(1)
C(35B)	1715(2)	1819(2)	1811(1)	32(1)
C(36B)	2173(2)	3909(2)	1785(1)	35(1)
C(37B)	1890(2)	3563(2)	2485(1)	34(1)
O(1C)	7650(2)	5619(1)	9974(1)	33(1)
C(1C)	8500(3)	6158(2)	10621(1)	47(1)
C(2C)	7669(2)	6212(2)	10264(1)	37(1)
C(3C)	6941(2)	5681(2)	9596(1)	35(1)
C(4C)	6891(3)	5000(2)	9329(2)	45(1)
O(1D)	5000	10000	0	78(2)
C(1D)	5801(5)	9798(4)	751(3)	105(3)
C(2E)	5803(7)	10128(5)	409(4)	70(3)
C(2D)	4961(9)	10361(6)	-312(4)	72(3)

Table 3. Selected bond lengths [Å] and angles [°] for IAT10 (CCDC 693797).

Ta(1)-O(2A)	1.9208(18)	Ta(2)-O(2B)	1.9161(16)
Ta(1)-O(1A)	1.9284(17)	Ta(2)-O(1B)	1.9232(15)
Ta(1)-N(2A)	1.9708(19)	Ta(2)-N(3B)	1.977(2)
Ta(1)-N(3A)	1.9847(19)	Ta(2)-N(2B)	1.9778(19)
Ta(1)-N(1A)	2.3921(17)	Ta(2)-N(1B)	2.4017(17)
Ta(1)-Cl(1A)	2.4686(6)	Ta(2)-Cl(1B)	2.4655(6)
O(2A)-Ta(1)-O(1A)	161.09(7)	O(2B)-Ta(2)-O(1B)	161.38(7)
O(2A)-Ta(1)-N(2A)	98.16(8)	O(2B)-Ta(2)-N(3B)	93.02(8)
O(1A)-Ta(1)-N(2A)	99.78(8)	O(1B)-Ta(2)-N(3B)	90.37(8)
O(2A)-Ta(1)-N(3A)	89.07(8)	O(2B)-Ta(2)-N(2B)	99.60(8)
O(1A)-Ta(1)-N(3A)	94.94(8)	O(1B)-Ta(2)-N(2B)	98.15(8)
N(2A)-Ta(1)-N(3A)	95.97(9)	N(3B)-Ta(2)-N(2B)	96.98(9)
O(2A)-Ta(1)-N(1A)	81.05(6)	O(2B)-Ta(2)-N(1B)	81.43(6)
O(1A)-Ta(1)-N(1A)	80.95(6)	O(1B)-Ta(2)-N(1B)	80.76(6)
N(2A)-Ta(1)-N(1A)	179.07(9)	N(3B)-Ta(2)-N(1B)	83.55(7)
N(3A)-Ta(1)-N(1A)	84.53(7)	N(2B)-Ta(2)-N(1B)	178.80(7)
O(2A)-Ta(1)-Cl(1A)	85.46(5)	O(2B)-Ta(2)-Cl(1B)	85.60(5)
O(1A)-Ta(1)-Cl(1A)	86.70(5)	O(1B)-Ta(2)-Cl(1B)	86.41(5)
N(2A)-Ta(1)-Cl(1A)	96.26(7)	N(3B)-Ta(2)-Cl(1B)	165.02(6)
N(3A)-Ta(1)-Cl(1A)	167.19(6)	N(2B)-Ta(2)-Cl(1B)	97.96(7)
N(1A)-Ta(1)-Cl(1A)	83.19(4)	N(1B)-Ta(2)-Cl(1B)	81.49(4)

Table 4. Bond lengths [Å] and angles [°] for IAT10 (CCDC 693797).

Ta(1)-O(2A)	1.9208(18)	Ta(2)-N(2B)	1.9778(19)
Ta(1)-O(1A)	1.9284(17)	Ta(2)-N(1B)	2.4017(17)
Ta(1)-N(2A)	1.9708(19)	Ta(2)-Cl(1B)	2.4655(6)
Ta(1)-N(3A)	1.9847(19)	O(1B)-C(1B)	1.343(2)
Ta(1)-N(1A)	2.3921(17)	O(2B)-C(17B)	1.339(3)
Ta(1)-Cl(1A)	2.4686(6)	N(1B)-C(11B)	1.359(3)
O(1A)-C(1A)	1.352(3)	N(1B)-C(7B)	1.364(3)
O(2A)-C(17A)	1.354(3)	N(2B)-C(34B)	1.461(4)
N(1A)-C(7A)	1.364(3)	N(2B)-C(35B)	1.467(4)
N(1A)-C(11A)	1.365(3)	N(3B)-C(36B)	1.453(3)
N(2A)-C(35A)	1.446(3)	N(3B)-C(37B)	1.467(3)
N(2A)-C(34A)	1.470(3)	C(1B)-C(6B)	1.397(3)
N(3A)-C(37A)	1.459(4)	C(1B)-C(2B)	1.413(3)
N(3A)-C(36A)	1.461(4)	C(2B)-C(3B)	1.393(3)
C(1A)-C(6A)	1.385(3)	C(2B)-C(18B)	1.541(3)
C(1A)-C(2A)	1.420(3)	C(3B)-C(4B)	1.395(3)
C(2A)-C(3A)	1.398(3)	C(4B)-C(5B)	1.386(3)
C(2A)-C(18A)	1.525(3)	C(4B)-C(22B)	1.532(3)
C(3A)-C(4A)	1.398(4)	C(5B)-C(6B)	1.398(3)
C(4A)-C(5A)	1.375(3)	C(6B)-C(7B)	1.483(3)
C(4A)-C(22A)	1.528(3)	C(7B)-C(8B)	1.397(3)
C(5A)-C(6A)	1.408(3)	C(8B)-C(9B)	1.379(3)
C(6A)-C(7A)	1.479(3)	C(9B)-C(10B)	1.385(3)
C(7A)-C(8A)	1.396(3)	C(10B)-C(11B)	1.390(3)
C(8A)-C(9A)	1.380(3)	C(11B)-C(12B)	1.482(3)
C(9A)-C(10A)	1.384(3)	C(12B)-C(17B)	1.397(3)
C(10A)-C(11A)	1.395(3)	C(12B)-C(13B)	1.396(4)
C(11A)-C(12A)	1.480(3)	C(13B)-C(14B)	1.387(3)
C(12A)-C(13A)	1.398(3)	C(14B)-C(15B)	1.390(3)
C(12A)-C(17A)	1.403(3)	C(14B)-C(26B)	1.536(4)
C(13A)-C(14A)	1.389(3)	C(15B)-C(16B)	1.396(4)
C(14A)-C(15A)	1.399(4)	C(16B)-C(17B)	1.414(3)
C(14A)-C(26A)	1.539(4)	C(16B)-C(30B)	1.534(3)
C(15A)-C(16A)	1.394(4)	C(18B)-C(19B)	1.536(4)
C(16A)-C(17A)	1.403(3)	C(18B)-C(21B)	1.539(4)
C(16A)-C(30A)	1.541(3)	C(18B)-C(20B)	1.543(4)
C(18A)-C(19A)	1.536(4)	C(22B)-C(23B)	1.529(3)
C(18A)-C(20A)	1.540(4)	C(22B)-C(25B)	1.528(4)
C(18A)-C(21A)	1.547(4)	C(22B)-C(24B)	1.532(4)
C(22A)-C(24A)	1.531(4)	C(26B)-C(27B)	1.520(5)
C(22A)-C(25A)	1.532(5)	C(26B)-C(28B)	1.523(4)
C(22A)-C(23A)	1.537(4)	C(26B)-C(29B)	1.531(6)
C(26A)-C(29A)	1.496(5)	C(30B)-C(33B)	1.524(4)
C(26A)-C(28A)	1.500(4)	C(30B)-C(31B)	1.538(4)
C(26A)-C(27A)	1.590(6)	C(30B)-C(32B)	1.546(4)
C(30A)-C(33A)	1.528(4)	O(1C)-C(2C)	1.410(4)
C(30A)-C(31A)	1.535(5)	O(1C)-C(3C)	1.410(4)
C(30A)-C(32A)	1.547(4)	C(1C)-C(2C)	1.481(5)
Ta(2)-O(2B)	1.9161(16)	C(3C)-C(4C)	1.496(5)
Ta(2)-O(1B)	1.9232(15)	O(1D)-C(2D)#1	1.171(10)
Ta(2)-N(3B)	1.977(2)	O(1D)-C(2D)	1.171(10)

O(1D)-C(2E)#1	1.570(13)	C(10A)-C(11A)-C(12A)	118.31(19)
O(1D)-C(2E)	1.570(13)	C(13A)-C(12A)-C(17A)	119.2(2)
C(1D)-C(2E)	1.226(13)	C(13A)-C(12A)-C(11A)	117.93(19)
C(1D)-C(2D)#1	1.609(14)	C(17A)-C(12A)-C(11A)	122.8(2)
C(2D)-C(1D)#1	1.609(14)	C(14A)-C(13A)-C(12A)	121.6(2)
		C(13A)-C(14A)-C(15A)	117.3(2)
O(2A)-Ta(1)-O(1A)	161.09(7)	C(13A)-C(14A)-C(26A)	120.1(2)
O(2A)-Ta(1)-N(2A)	98.16(8)	C(15A)-C(14A)-C(26A)	122.6(2)
O(1A)-Ta(1)-N(2A)	99.78(8)	C(16A)-C(15A)-C(14A)	123.7(2)
O(2A)-Ta(1)-N(3A)	89.07(8)	C(15A)-C(16A)-C(17A)	117.1(2)
O(1A)-Ta(1)-N(3A)	94.94(8)	C(15A)-C(16A)-C(30A)	121.5(2)
N(2A)-Ta(1)-N(3A)	95.97(9)	C(17A)-C(16A)-C(30A)	121.5(2)
O(2A)-Ta(1)-N(1A)	81.05(6)	O(2A)-C(17A)-C(12A)	117.7(2)
O(1A)-Ta(1)-N(1A)	80.95(6)	O(2A)-C(17A)-C(16A)	121.18(19)
N(2A)-Ta(1)-N(1A)	179.07(9)	C(12A)-C(17A)-C(16A)	121.1(2)
N(3A)-Ta(1)-N(1A)	84.53(7)	C(2A)-C(18A)-C(19A)	108.6(2)
O(2A)-Ta(1)-Cl(1A)	85.46(5)	C(2A)-C(18A)-C(20A)	111.8(2)
O(1A)-Ta(1)-Cl(1A)	86.70(5)	C(19A)-C(18A)-C(20A)	107.8(2)
N(2A)-Ta(1)-Cl(1A)	96.26(7)	C(2A)-C(18A)-C(21A)	111.2(2)
N(3A)-Ta(1)-Cl(1A)	167.19(6)	C(19A)-C(18A)-C(21A)	110.7(2)
N(1A)-Ta(1)-Cl(1A)	83.19(4)	C(20A)-C(18A)-C(21A)	106.7(2)
C(1A)-O(1A)-Ta(1)	141.00(15)	C(4A)-C(22A)-C(24A)	109.0(2)
C(17A)-O(2A)-Ta(1)	137.93(13)	C(4A)-C(22A)-C(25A)	110.3(2)
C(7A)-N(1A)-C(11A)	118.38(17)	C(24A)-C(22A)-C(25A)	111.0(3)
C(7A)-N(1A)-Ta(1)	117.22(14)	C(4A)-C(22A)-C(23A)	112.8(2)
C(11A)-N(1A)-Ta(1)	117.68(13)	C(24A)-C(22A)-C(23A)	107.0(3)
C(35A)-N(2A)-C(34A)	110.8(2)	C(25A)-C(22A)-C(23A)	106.6(3)
C(35A)-N(2A)-Ta(1)	126.50(18)	C(29A)-C(26A)-C(28A)	112.8(3)
C(34A)-N(2A)-Ta(1)	122.52(17)	C(29A)-C(26A)-C(14A)	110.5(3)
C(37A)-N(3A)-C(36A)	109.8(2)	C(28A)-C(26A)-C(14A)	112.9(3)
C(37A)-N(3A)-Ta(1)	128.1(2)	C(29A)-C(26A)-C(27A)	107.9(4)
C(36A)-N(3A)-Ta(1)	121.83(17)	C(28A)-C(26A)-C(27A)	104.7(3)
O(1A)-C(1A)-C(6A)	118.75(19)	C(14A)-C(26A)-C(27A)	107.6(3)
O(1A)-C(1A)-C(2A)	119.82(19)	C(33A)-C(30A)-C(31A)	107.8(3)
C(6A)-C(1A)-C(2A)	121.4(2)	C(33A)-C(30A)-C(16A)	111.8(2)
C(3A)-C(2A)-C(1A)	116.0(2)	C(31A)-C(30A)-C(16A)	110.5(2)
C(3A)-C(2A)-C(18A)	121.4(2)	C(33A)-C(30A)-C(32A)	107.5(2)
C(1A)-C(2A)-C(18A)	122.6(2)	C(31A)-C(30A)-C(32A)	110.4(3)
C(4A)-C(3A)-C(2A)	124.4(2)	C(16A)-C(30A)-C(32A)	108.8(2)
C(5A)-C(4A)-C(3A)	116.9(2)	O(2B)-Ta(2)-O(1B)	161.38(7)
C(5A)-C(4A)-C(22A)	123.2(2)	O(2B)-Ta(2)-N(3B)	93.02(8)
C(3A)-C(4A)-C(22A)	119.9(2)	O(1B)-Ta(2)-N(3B)	90.37(8)
C(4A)-C(5A)-C(6A)	122.1(2)	O(2B)-Ta(2)-N(2B)	99.60(8)
C(1A)-C(6A)-C(5A)	119.1(2)	O(1B)-Ta(2)-N(2B)	98.15(8)
C(1A)-C(6A)-C(7A)	123.80(19)	N(3B)-Ta(2)-N(2B)	96.98(9)
C(5A)-C(6A)-C(7A)	117.03(19)	O(2B)-Ta(2)-N(1B)	81.43(6)
N(1A)-C(7A)-C(8A)	120.76(19)	O(1B)-Ta(2)-N(1B)	80.76(6)
N(1A)-C(7A)-C(6A)	120.49(18)	N(3B)-Ta(2)-N(1B)	83.55(7)
C(8A)-C(7A)-C(6A)	118.49(19)	N(2B)-Ta(2)-N(1B)	178.80(7)
C(9A)-C(8A)-C(7A)	120.2(2)	O(2B)-Ta(2)-Cl(1B)	85.60(5)
C(8A)-C(9A)-C(10A)	118.5(2)	O(1B)-Ta(2)-Cl(1B)	86.41(5)
C(9A)-C(10A)-C(11A)	119.8(2)	N(3B)-Ta(2)-Cl(1B)	165.02(6)
N(1A)-C(11A)-C(10A)	121.1(2)	N(2B)-Ta(2)-Cl(1B)	97.96(7)
N(1A)-C(11A)-C(12A)	120.41(18)	N(1B)-Ta(2)-Cl(1B)	81.49(4)

C(1B)-O(1B)-Ta(2)	139.65(15)	C(13B)-C(14B)-C(26B)	120.4(2)
C(17B)-O(2B)-Ta(2)	140.64(13)	C(15B)-C(14B)-C(26B)	121.9(2)
C(11B)-N(1B)-C(7B)	118.23(17)	C(14B)-C(15B)-C(16B)	123.5(2)
C(11B)-N(1B)-Ta(2)	117.13(12)	C(15B)-C(16B)-C(17B)	116.8(2)
C(7B)-N(1B)-Ta(2)	117.47(14)	C(15B)-C(16B)-C(30B)	121.9(2)
C(34B)-N(2B)-C(35B)	110.1(2)	C(17B)-C(16B)-C(30B)	121.3(2)
C(34B)-N(2B)-Ta(2)	125.3(2)	O(2B)-C(17B)-C(12B)	118.92(19)
C(35B)-N(2B)-Ta(2)	124.52(18)	O(2B)-C(17B)-C(16B)	119.93(19)
C(36B)-N(3B)-C(37B)	110.0(2)	C(12B)-C(17B)-C(16B)	121.1(2)
C(36B)-N(3B)-Ta(2)	126.93(16)	C(19B)-C(18B)-C(21B)	108.1(2)
C(37B)-N(3B)-Ta(2)	122.69(18)	C(19B)-C(18B)-C(2B)	111.4(2)
O(1B)-C(1B)-C(6B)	118.32(18)	C(21B)-C(18B)-C(2B)	108.9(2)
O(1B)-C(1B)-C(2B)	120.37(19)	C(19B)-C(18B)-C(20B)	107.2(3)
C(6B)-C(1B)-C(2B)	121.28(18)	C(21B)-C(18B)-C(20B)	109.7(2)
C(3B)-C(2B)-C(1B)	116.8(2)	C(2B)-C(18B)-C(20B)	111.6(2)
C(3B)-C(2B)-C(18B)	121.54(19)	C(23B)-C(22B)-C(25B)	109.3(2)
C(1B)-C(2B)-C(18B)	121.58(19)	C(23B)-C(22B)-C(4B)	110.41(19)
C(2B)-C(3B)-C(4B)	123.6(2)	C(25B)-C(22B)-C(4B)	108.8(2)
C(5B)-C(4B)-C(3B)	117.50(18)	C(23B)-C(22B)-C(24B)	107.7(2)
C(5B)-C(4B)-C(22B)	122.2(2)	C(25B)-C(22B)-C(24B)	108.8(2)
C(3B)-C(4B)-C(22B)	120.29(19)	C(4B)-C(22B)-C(24B)	111.82(18)
C(4B)-C(5B)-C(6B)	121.8(2)	C(27B)-C(26B)-C(28B)	107.8(3)
C(1B)-C(6B)-C(5B)	118.92(18)	C(27B)-C(26B)-C(29B)	111.1(4)
C(1B)-C(6B)-C(7B)	123.38(17)	C(28B)-C(26B)-C(29B)	106.4(3)
C(5B)-C(6B)-C(7B)	117.60(18)	C(27B)-C(26B)-C(14B)	109.0(3)
N(1B)-C(7B)-C(8B)	121.11(19)	C(28B)-C(26B)-C(14B)	112.3(2)
N(1B)-C(7B)-C(6B)	119.97(16)	C(29B)-C(26B)-C(14B)	110.3(3)
C(8B)-C(7B)-C(6B)	118.67(17)	C(33B)-C(30B)-C(16B)	111.6(2)
C(9B)-C(8B)-C(7B)	119.94(19)	C(33B)-C(30B)-C(31B)	106.9(2)
C(8B)-C(9B)-C(10B)	118.3(2)	C(16B)-C(30B)-C(31B)	112.7(2)
C(9B)-C(10B)-C(11B)	120.0(2)	C(33B)-C(30B)-C(32B)	107.9(2)
N(1B)-C(11B)-C(10B)	121.34(19)	C(16B)-C(30B)-C(32B)	107.9(2)
N(1B)-C(11B)-C(12B)	120.74(17)	C(31B)-C(30B)-C(32B)	109.8(3)
C(10B)-C(11B)-C(12B)	117.81(19)	C(2C)-O(1C)-C(3C)	112.9(2)
C(17B)-C(12B)-C(13B)	119.1(2)	O(1C)-C(2C)-C(1C)	109.6(3)
C(17B)-C(12B)-C(11B)	123.0(2)	O(1C)-C(3C)-C(4C)	110.1(3)
C(13B)-C(12B)-C(11B)	117.95(19)	C(2D)-O(1D)-C(2E)	119.6(7)
C(14B)-C(13B)-C(12B)	121.6(2)	C(1D)-C(2E)-O(1D)	119.9(7)
C(13B)-C(14B)-C(15B)	117.8(2)	O(1D)-C(2D)-C(1D)#1	120.8(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT10 (CCDC 693797). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	128(1)	153(1)	150(1)	-23(1)	10(1)	9(1)
Cl(1A)	179(2)	175(2)	263(3)	10(2)	29(2)	-28(2)
O(1A)	175(7)	161(6)	163(7)	8(5)	-17(5)	24(5)
O(2A)	166(7)	242(7)	148(7)	-29(6)	39(6)	16(6)
N(1A)	121(7)	163(6)	102(7)	6(5)	10(6)	-1(5)
N(2A)	207(10)	213(8)	246(11)	-47(7)	14(8)	31(7)
N(3A)	144(9)	237(8)	232(10)	-44(7)	44(7)	-27(6)
C(1A)	153(9)	179(7)	132(9)	19(6)	10(7)	-8(6)
C(2A)	204(11)	198(8)	179(10)	38(7)	-2(8)	-26(7)
C(3A)	222(11)	283(11)	164(10)	54(8)	11(8)	-44(8)
C(4A)	188(11)	310(10)	137(10)	10(8)	40(8)	-20(8)
C(5A)	170(10)	240(9)	132(9)	-5(7)	18(7)	-7(7)
C(6A)	156(9)	183(8)	116(8)	5(6)	9(7)	-12(6)
C(7A)	122(8)	173(7)	127(8)	1(6)	21(7)	2(6)
C(8A)	213(11)	166(8)	159(10)	-21(7)	-4(8)	15(7)
C(9A)	262(12)	151(8)	201(11)	-1(7)	-31(9)	16(7)
C(10A)	238(11)	166(8)	168(10)	42(7)	-20(8)	12(7)
C(11A)	137(9)	165(7)	111(8)	15(6)	5(7)	8(6)
C(12A)	158(9)	197(8)	107(8)	14(6)	12(7)	-26(7)
C(13A)	185(10)	216(8)	128(9)	32(7)	-1(7)	-19(7)
C(14A)	202(11)	245(9)	159(10)	51(7)	-22(8)	-43(8)
C(15A)	242(12)	305(11)	123(10)	-11(8)	-4(8)	-60(9)
C(16A)	191(10)	273(10)	134(9)	-47(8)	24(8)	-31(8)
C(17A)	152(9)	225(8)	128(9)	-13(7)	37(7)	-20(7)
C(18A)	304(13)	210(9)	190(11)	56(8)	-14(9)	-17(8)
C(19A)	365(16)	223(10)	279(14)	27(9)	-21(11)	-45(10)
C(20A)	472(19)	314(12)	230(14)	106(10)	-32(12)	37(12)
C(21A)	288(14)	262(11)	323(15)	66(10)	13(11)	64(9)
C(22A)	254(13)	413(13)	148(11)	10(9)	73(9)	6(10)
C(23A)	358(16)	374(13)	219(13)	-81(10)	115(12)	-11(11)
C(24A)	570(20)	421(16)	600(30)	67(15)	440(20)	-14(15)
C(25A)	420(20)	870(30)	146(13)	-71(15)	26(13)	199(18)
C(26A)	319(15)	255(11)	323(15)	51(10)	-182(11)	-34(10)
C(27A)	327(19)	650(20)	510(20)	-155(19)	-80(16)	167(16)
C(28A)	291(16)	512(18)	319(17)	-86(14)	-136(12)	34(13)
C(29A)	840(40)	630(30)	1190(50)	680(30)	-660(30)	-370(30)
C(30A)	257(12)	395(12)	202(11)	-122(11)	24(9)	14(11)
C(31A)	344(16)	303(12)	317(16)	-118(11)	10(12)	64(11)
C(32A)	288(15)	630(20)	289(15)	-152(13)	113(13)	29(13)
C(33A)	406(19)	556(19)	255(15)	-221(13)	-6(13)	39(14)
C(34A)	241(13)	347(13)	382(17)	-122(11)	86(12)	50(10)
C(35A)	371(16)	207(10)	441(19)	-61(10)	63(14)	60(10)
C(36A)	175(12)	407(14)	313(15)	10(11)	-11(10)	-68(10)
C(37A)	290(15)	485(17)	345(17)	89(13)	49(13)	-146(13)

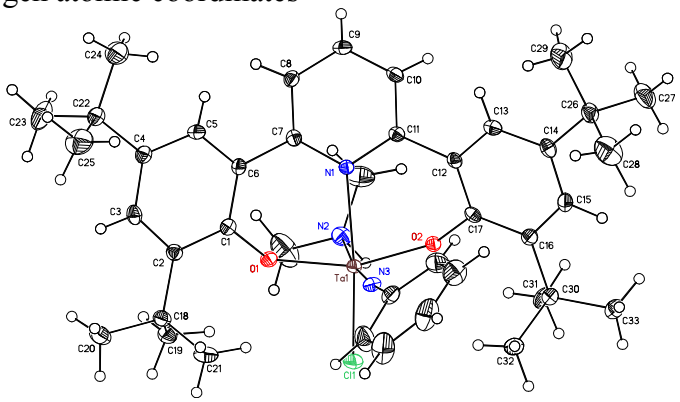
Ta(2)	125(1)	143(1)	140(1)	4(1)	31(1)	-28(1)
Cl(1B)	204(3)	179(2)	348(3)	32(2)	46(2)	37(2)
O(1B)	156(7)	186(6)	134(7)	17(5)	30(6)	-26(5)
O(2B)	181(7)	204(6)	142(7)	15(6)	20(5)	-47(6)
N(1B)	151(8)	145(6)	107(7)	10(5)	38(6)	-6(5)
N(2B)	232(10)	246(8)	198(10)	-28(7)	67(8)	-104(7)
N(3B)	145(9)	245(8)	217(10)	32(7)	45(7)	22(6)
C(1B)	146(9)	191(8)	130(9)	18(6)	21(7)	-15(6)
C(2B)	213(11)	212(8)	135(9)	-15(7)	45(8)	-28(7)
C(3B)	205(11)	232(9)	132(9)	-11(7)	51(8)	-15(7)
C(4B)	148(9)	211(8)	123(9)	30(6)	26(7)	-1(7)
C(5B)	152(9)	176(7)	116(8)	28(6)	19(7)	-6(6)
C(6B)	134(8)	161(7)	108(8)	28(6)	17(7)	6(6)
C(7B)	117(8)	144(7)	142(9)	14(6)	29(7)	-3(6)
C(8B)	228(11)	144(7)	180(10)	32(7)	73(8)	-1(7)
C(9B)	318(13)	148(8)	230(12)	-4(7)	113(10)	-24(8)
C(10B)	304(13)	173(8)	164(10)	-30(7)	95(9)	-49(8)
C(11B)	174(9)	157(7)	119(8)	2(6)	41(7)	-36(6)
C(12B)	195(10)	199(8)	125(9)	11(7)	35(8)	-37(7)
C(13B)	228(11)	257(10)	163(10)	13(8)	14(9)	-72(8)
C(14B)	237(12)	303(11)	137(10)	21(8)	9(9)	-23(9)
C(15B)	235(11)	271(10)	144(9)	44(7)	23(8)	-14(8)
C(16B)	211(11)	213(8)	157(10)	48(7)	36(8)	-20(7)
C(17B)	203(10)	180(8)	101(8)	16(6)	38(7)	-22(7)
C(18B)	296(13)	213(10)	203(11)	-43(7)	69(10)	-49(8)
C(19B)	630(20)	367(14)	297(16)	-166(12)	226(16)	-193(15)
C(20B)	301(14)	236(11)	304(14)	-35(9)	-68(11)	-42(9)
C(21B)	295(14)	219(10)	291(14)	-38(9)	20(11)	9(9)
C(22B)	162(10)	251(9)	130(9)	36(7)	40(7)	-11(7)
C(23B)	225(13)	375(13)	418(18)	51(12)	151(13)	54(10)
C(24B)	266(14)	429(14)	226(13)	-2(10)	81(11)	-151(11)
C(25B)	277(13)	349(12)	171(11)	99(9)	33(10)	-13(10)
C(26B)	281(14)	448(15)	155(11)	13(10)	-21(10)	-105(11)
C(27B)	300(20)	1700(60)	370(20)	-220(30)	-11(17)	-200(30)
C(28B)	420(20)	690(20)	178(14)	35(14)	-43(12)	-106(16)
C(29B)	1390(50)	500(20)	320(20)	8(17)	-320(30)	-390(30)
C(30B)	310(14)	247(10)	206(12)	87(8)	48(10)	-44(9)
C(31B)	284(14)	400(14)	350(16)	136(12)	66(12)	-103(11)
C(32B)	490(19)	208(10)	307(15)	57(9)	74(13)	-9(11)
C(33B)	466(19)	377(14)	242(14)	121(11)	59(13)	-127(13)
C(34B)	393(17)	212(10)	500(20)	-37(11)	104(15)	-107(11)
C(35B)	280(14)	378(14)	280(14)	-41(11)	6(11)	-137(11)
C(36B)	271(14)	480(16)	305(16)	162(12)	61(12)	177(12)
C(37B)	271(14)	444(15)	341(16)	73(12)	153(13)	129(12)
O(1C)	242(10)	313(9)	434(14)	68(8)	82(9)	37(7)
C(1C)	364(19)	630(20)	430(20)	120(17)	104(16)	-101(16)
C(2C)	331(17)	372(14)	425(19)	67(13)	103(14)	1(12)
C(3C)	271(15)	345(13)	428(19)	100(12)	79(13)	38(11)
C(4C)	390(20)	400(16)	570(30)	-63(15)	88(18)	14(14)
O(1D)	530(30)	550(30)	1270(60)	0(30)	210(30)	-190(20)

C(1D)	640(40)	1050(50)	1450(80)	-310(50)	210(50)	-70(40)
C(2E)	660(70)	450(40)	1120(100)	20(50)	460(70)	-170(40)
C(2D)	1100(100)	630(50)	540(60)	90(50)	380(70)	-80(60)

Crystal Structure Analysis of:

Complex 4 (IAT16)

Contents



IAT16

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 694413. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 694413."

Table 1. Crystal data and structure refinement for IAT16 (CCDC 694413).

Empirical formula	$C_{41}H_{55}N_3O_2ClTa$
Formula weight	838.28
Crystallization Solvent	Benzene
Crystal Habit	Block
Crystal size	0.09 x 0.09 x 0.06 mm^3
Crystal color	Yellow

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9137 reflections used in lattice determination	2.18 to 34.73°	
Unit cell dimensions	a = 9.9628(5) Å b = 10.6118(5) Å c = 18.9240(9) Å	α= 80.804(3)° β= 89.355(3)° γ = 81.578(3)°
Volume	1953.54(16) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.425 Mg/m^3	
F(000)	856	
Data collection program	Bruker APEX2 v2.1-0	
θ range for data collection	1.97 to 35.14°	
Completeness to θ = 35.14°	90.5 %	
Index ranges	$-15 \le h \le 14$, $-17 \le k \le 17$, $-29 \le l \le 30$	
Data collection scan type	ω scans; 15 settings	
Data reduction program	Bruker SAINT-Plus v7.34A	
Reflections collected	58512	
Independent reflections	15730 [R_{int}= 0.0505]	
Absorption coefficient	2.919 mm^{-1}	
Absorption correction	None	
Max. and min. transmission	0.8444 and 0.7791	

Table 1 (cont.)

Structure solution and Refinement

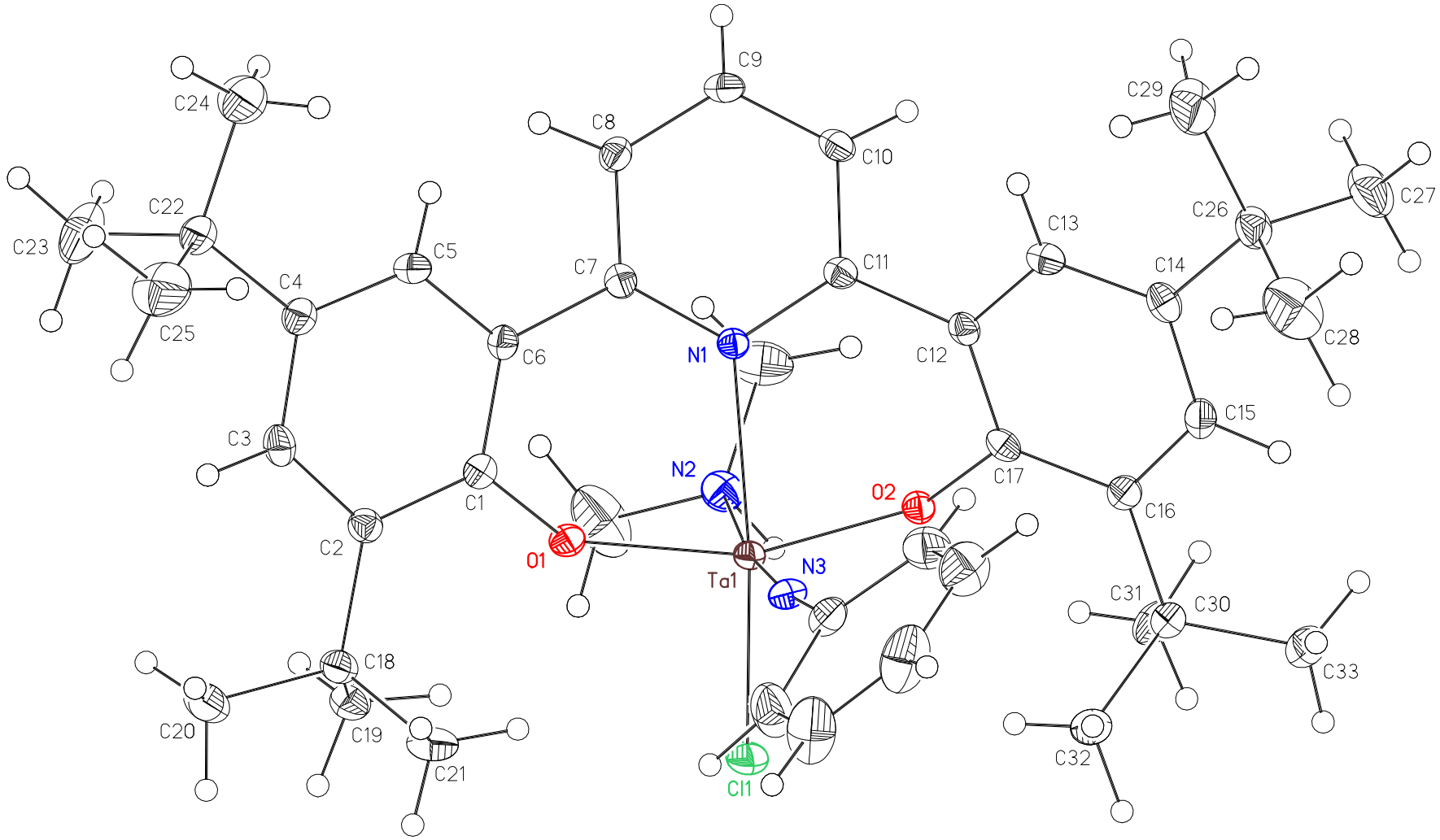
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	15730 / 0 / 653
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.281
Final R indices [$I>2\sigma(I)$, 12866 reflections]	R1 = 0.0326, *w*R2 = 0.0452
R indices (all data)	R1 = 0.0473, *w*R2 = 0.0462
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.005
Average shift/error	0.000
Largest diff. peak and hole	3.936 and -2.313 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C9
C24
C8
C10
C29
C22
C23
C5
C7
C11
C13
C26
C27
C4
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C12
C14
C28
C3
C15
N2
C17
O2
C1
C16
O1
Ta1
N3
C2
C31
C30
C18
C33
C20
C19
C32
C21
Cl1

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT16 (CCDC 694413). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	7043(1)	5812(1)	7129(1)	12(1)
Cl(1)	4834(1)	6355(1)	6585(1)	22(1)
O(1)	6600(1)	6836(1)	7887(1)	15(1)
O(2)	8002(1)	5393(1)	6265(1)	13(1)
N(1)	9195(2)	5883(1)	7519(1)	11(1)
N(2)	7282(2)	7912(2)	6415(1)	19(1)
N(3)	7006(2)	4203(2)	7574(1)	15(1)
C(1)	7100(2)	6937(2)	8525(1)	13(1)
C(2)	6231(2)	7166(2)	9105(1)	14(1)
C(3)	6844(2)	7293(2)	9738(1)	16(1)
C(4)	8248(2)	7200(2)	9841(1)	15(1)
C(5)	9048(2)	6980(2)	9258(1)	16(1)
C(6)	8508(2)	6859(2)	8600(1)	13(1)
C(7)	9455(2)	6638(2)	8008(1)	13(1)
C(8)	10672(2)	7145(2)	7991(1)	14(1)
C(9)	11680(2)	6782(2)	7532(1)	16(1)
C(10)	11495(2)	5878(2)	7118(1)	15(1)
C(11)	10257(2)	5424(2)	7119(1)	12(1)
C(12)	10140(2)	4385(2)	6699(1)	12(1)
C(13)	11231(2)	3378(2)	6732(1)	14(1)
C(14)	11219(2)	2391(2)	6342(1)	15(1)
C(15)	10086(2)	2449(2)	5898(1)	16(1)
C(16)	8972(2)	3421(2)	5838(1)	14(1)
C(17)	9020(2)	4388(2)	6263(1)	12(1)
C(18)	4685(2)	7272(2)	9021(1)	17(1)
C(19)	4162(2)	8330(2)	8395(1)	20(1)
C(20)	3948(2)	7620(3)	9690(1)	28(1)
C(21)	4322(2)	5966(2)	8896(1)	22(1)
C(22)	8829(2)	7380(2)	10555(1)	21(1)
C(23)	8341(3)	8760(3)	10686(2)	39(1)
C(24)	10381(3)	7146(4)	10570(2)	42(1)
C(25)	8346(3)	6433(3)	11162(2)	36(1)
C(26)	12398(2)	1272(2)	6381(1)	19(1)
C(27)	13047(3)	1284(3)	5647(2)	31(1)
C(28)	11870(3)	-9(2)	6603(2)	38(1)
C(29)	13492(3)	1397(3)	6913(2)	35(1)
C(30)	7748(2)	3415(2)	5358(1)	16(1)
C(31)	7468(3)	4699(2)	4843(1)	23(1)
C(32)	6496(2)	3211(2)	5812(1)	23(1)
C(33)	7976(3)	2343(2)	4903(1)	25(1)
C(34)	6497(3)	9027(3)	6655(2)	44(1)
C(35)	8658(3)	8176(3)	6214(2)	30(1)
C(36)	7087(2)	2919(2)	7876(1)	18(1)
C(37)	6059(3)	2497(2)	8313(1)	31(1)
C(38)	6162(3)	1211(2)	8623(2)	40(1)
C(39)	7270(3)	349(2)	8510(1)	35(1)
C(40)	8275(3)	736(2)	8063(1)	30(1)
C(41)	8186(2)	2009(2)	7744(1)	24(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT16 (CCDC 694413).

Ta(1)-N(3)	1.7840(15)	N(3)-Ta(1)-O(1)	102.94(7)
Ta(1)-O(1)	1.9438(14)	N(3)-Ta(1)-O(2)	98.12(7)
Ta(1)-O(2)	1.9643(13)	O(1)-Ta(1)-O(2)	154.01(5)
Ta(1)-N(1)	2.2918(16)	N(3)-Ta(1)-N(1)	94.12(6)
Ta(1)-Cl(1)	2.3920(5)	O(1)-Ta(1)-N(1)	80.82(6)
Ta(1)-N(2)	2.4569(17)	O(2)-Ta(1)-N(1)	82.66(6)
		N(3)-Ta(1)-Cl(1)	102.00(5)
		O(1)-Ta(1)-Cl(1)	94.23(4)
		O(2)-Ta(1)-Cl(1)	96.12(4)
		N(1)-Ta(1)-Cl(1)	163.84(4)
		N(3)-Ta(1)-N(2)	173.15(7)
		O(1)-Ta(1)-N(2)	83.24(6)
		O(2)-Ta(1)-N(2)	75.15(6)
		N(1)-Ta(1)-N(2)	83.86(6)
		Cl(1)-Ta(1)-N(2)	80.26(5)

Table 4. Bond lengths [Å] and angles [°] for IAT16 (CCDC 694413).

Ta(1)-N(3)	1.7840(15)	C(21)-H(21A)	0.85(2)
Ta(1)-O(1)	1.9438(14)	C(21)-H(21B)	0.96(2)
Ta(1)-O(2)	1.9643(13)	C(21)-H(21C)	0.88(2)
Ta(1)-N(1)	2.2918(16)	C(22)-C(25)	1.524(3)
Ta(1)-Cl(1)	2.3920(5)	C(22)-C(24)	1.530(3)
Ta(1)-N(2)	2.4569(17)	C(22)-C(23)	1.532(3)
O(1)-C(1)	1.336(2)	C(23)-H(23A)	0.97(3)
O(2)-C(17)	1.360(2)	C(23)-H(23B)	0.98(3)
N(1)-C(7)	1.367(2)	C(23)-H(23C)	0.98(3)
N(1)-C(11)	1.371(2)	C(24)-H(24A)	1.01(3)
N(2)-C(34)	1.453(3)	C(24)-H(24B)	0.87(3)
N(2)-C(35)	1.472(3)	C(24)-H(24C)	1.07(3)
N(2)-H(2)	0.91(2)	C(25)-H(25A)	0.97(3)
N(3)-C(36)	1.382(2)	C(25)-H(25B)	1.00(3)
C(1)-C(6)	1.400(3)	C(25)-H(25C)	0.97(3)
C(1)-C(2)	1.420(3)	C(26)-C(29)	1.525(3)
C(2)-C(3)	1.386(3)	C(26)-C(27)	1.526(3)
C(2)-C(18)	1.536(3)	C(26)-C(28)	1.524(3)
C(3)-C(4)	1.401(3)	C(27)-H(27A)	1.04(3)
C(3)-H(3)	0.88(2)	C(27)-H(27B)	0.92(3)
C(4)-C(5)	1.383(3)	C(27)-H(27C)	0.86(2)
C(4)-C(22)	1.527(3)	C(28)-H(28A)	1.08(3)
C(5)-C(6)	1.395(3)	C(28)-H(28B)	0.91(3)
C(5)-H(5)	0.83(2)	C(28)-H(28C)	0.94(3)
C(6)-C(7)	1.481(3)	C(29)-H(29A)	0.89(2)
C(7)-C(8)	1.395(3)	C(29)-H(29B)	0.92(3)
C(8)-C(9)	1.373(3)	C(29)-H(29C)	1.03(2)
C(8)-H(8)	0.88(2)	C(30)-C(33)	1.523(3)
C(9)-C(10)	1.364(3)	C(30)-C(32)	1.529(3)
C(9)-H(9)	0.80(2)	C(30)-C(31)	1.535(3)
C(10)-C(11)	1.388(3)	C(31)-H(31A)	0.98(3)
C(10)-H(10)	0.83(2)	C(31)-H(31B)	0.85(2)
C(11)-C(12)	1.476(3)	C(31)-H(31C)	0.92(2)
C(12)-C(17)	1.395(3)	C(32)-H(32A)	1.02(2)
C(12)-C(13)	1.403(3)	C(32)-H(32B)	0.83(2)
C(13)-C(14)	1.377(3)	C(32)-H(32C)	0.95(2)
C(13)-H(13)	0.91(2)	C(33)-H(33A)	0.95(2)
C(14)-C(15)	1.403(3)	C(33)-H(33B)	0.90(2)
C(14)-C(26)	1.536(3)	C(33)-H(33C)	0.87(2)
C(15)-C(16)	1.393(3)	C(34)-H(34A)	1.09(2)
C(15)-H(15)	0.923(19)	C(34)-H(34B)	0.99(3)
C(16)-C(17)	1.408(3)	C(34)-H(34C)	0.88(3)
C(16)-C(30)	1.530(3)	C(35)-H(35A)	0.97(2)
C(18)-C(20)	1.524(3)	C(35)-H(35B)	1.01(3)
C(18)-C(19)	1.535(3)	C(35)-H(35C)	0.94(3)
C(18)-C(21)	1.536(3)	C(36)-C(37)	1.389(3)
C(19)-H(19A)	0.95(2)	C(36)-C(41)	1.398(3)
C(19)-H(19B)	1.00(2)	C(37)-C(38)	1.387(3)
C(19)-H(19C)	0.82(3)	C(37)-H(37)	0.99(2)
C(20)-H(20A)	0.92(2)	C(38)-C(39)	1.364(4)
C(20)-H(20B)	0.95(2)	C(38)-H(38)	0.87(3)
C(20)-H(20C)	0.91(2)	C(39)-C(40)	1.370(4)

C(39)-H(39)	0.83(2)	C(9)-C(8)-H(8)	125.4(13)
C(40)-C(41)	1.380(3)	C(7)-C(8)-H(8)	114.2(13)
C(40)-H(40)	0.87(2)	C(10)-C(9)-C(8)	119.0(2)
C(41)-H(41)	0.83(2)	C(10)-C(9)-H(9)	120.9(16)
		C(8)-C(9)-H(9)	120.1(16)
N(3)-Ta(1)-O(1)	102.94(7)	C(9)-C(10)-C(11)	119.9(2)
N(3)-Ta(1)-O(2)	98.12(7)	C(9)-C(10)-H(10)	124.7(15)
O(1)-Ta(1)-O(2)	154.01(5)	C(11)-C(10)-H(10)	115.2(15)
N(3)-Ta(1)-N(1)	94.12(6)	N(1)-C(11)-C(10)	121.29(19)
O(1)-Ta(1)-N(1)	80.82(6)	N(1)-C(11)-C(12)	120.91(17)
O(2)-Ta(1)-N(1)	82.66(6)	C(10)-C(11)-C(12)	117.74(18)
N(3)-Ta(1)-Cl(1)	102.00(5)	C(17)-C(12)-C(13)	119.46(19)
O(1)-Ta(1)-Cl(1)	94.23(4)	C(17)-C(12)-C(11)	122.92(17)
O(2)-Ta(1)-Cl(1)	96.12(4)	C(13)-C(12)-C(11)	117.60(18)
N(1)-Ta(1)-Cl(1)	163.84(4)	C(14)-C(13)-C(12)	121.26(19)
N(3)-Ta(1)-N(2)	173.15(7)	C(14)-C(13)-H(13)	120.5(13)
O(1)-Ta(1)-N(2)	83.24(6)	C(12)-C(13)-H(13)	118.2(13)
O(2)-Ta(1)-N(2)	75.15(6)	C(13)-C(14)-C(15)	117.32(18)
N(1)-Ta(1)-N(2)	83.86(6)	C(13)-C(14)-C(26)	121.75(19)
Cl(1)-Ta(1)-N(2)	80.26(5)	C(15)-C(14)-C(26)	120.93(19)
C(1)-O(1)-Ta(1)	138.20(12)	C(16)-C(15)-C(14)	124.4(2)
C(17)-O(2)-Ta(1)	124.00(11)	C(16)-C(15)-H(15)	114.1(12)
C(7)-N(1)-C(11)	117.76(17)	C(14)-C(15)-H(15)	121.5(12)
C(7)-N(1)-Ta(1)	122.51(12)	C(15)-C(16)-C(17)	115.99(19)
C(11)-N(1)-Ta(1)	117.58(13)	C(15)-C(16)-C(30)	122.00(18)
C(34)-N(2)-C(35)	110.5(2)	C(17)-C(16)-C(30)	121.98(17)
C(34)-N(2)-Ta(1)	115.65(16)	O(2)-C(17)-C(12)	115.83(18)
C(35)-N(2)-Ta(1)	118.09(14)	O(2)-C(17)-C(16)	122.59(18)
C(34)-N(2)-H(2)	102.3(16)	C(12)-C(17)-C(16)	121.57(17)
C(35)-N(2)-H(2)	108.8(15)	C(20)-C(18)-C(19)	107.24(18)
Ta(1)-N(2)-H(2)	99.4(14)	C(20)-C(18)-C(2)	111.79(18)
C(36)-N(3)-Ta(1)	174.17(15)	C(19)-C(18)-C(2)	110.49(17)
O(1)-C(1)-C(6)	118.15(17)	C(20)-C(18)-C(21)	107.74(19)
O(1)-C(1)-C(2)	121.24(18)	C(19)-C(18)-C(21)	110.21(19)
C(6)-C(1)-C(2)	120.56(19)	C(2)-C(18)-C(21)	109.32(17)
C(3)-C(2)-C(1)	116.91(19)	C(18)-C(19)-H(19A)	105.9(13)
C(3)-C(2)-C(18)	122.35(18)	C(18)-C(19)-H(19B)	109.2(11)
C(1)-C(2)-C(18)	120.74(18)	H(19A)-C(19)-H(19B)	113.1(19)
C(2)-C(3)-C(4)	124.4(2)	C(18)-C(19)-H(19C)	111.1(18)
C(2)-C(3)-H(3)	120.1(15)	H(19A)-C(19)-H(19C)	101(2)
C(4)-C(3)-H(3)	115.5(15)	H(19B)-C(19)-H(19C)	116(2)
C(5)-C(4)-C(3)	116.33(19)	C(18)-C(20)-H(20A)	111.8(13)
C(5)-C(4)-C(22)	122.98(19)	C(18)-C(20)-H(20B)	100.4(15)
C(3)-C(4)-C(22)	120.66(18)	H(20A)-C(20)-H(20B)	112.4(19)
C(4)-C(5)-C(6)	122.71(19)	C(18)-C(20)-H(20C)	112.3(14)
C(4)-C(5)-H(5)	120.0(15)	H(20A)-C(20)-H(20C)	110(2)
C(6)-C(5)-H(5)	117.2(15)	H(20B)-C(20)-H(20C)	109.2(19)
C(5)-C(6)-C(1)	119.04(18)	C(18)-C(21)-H(21A)	109.1(16)
C(5)-C(6)-C(7)	118.36(18)	C(18)-C(21)-H(21B)	111.5(12)
C(1)-C(6)-C(7)	122.60(18)	H(21A)-C(21)-H(21B)	112.5(19)
N(1)-C(7)-C(8)	120.40(18)	C(18)-C(21)-H(21C)	109.4(15)
N(1)-C(7)-C(6)	121.23(17)	H(21A)-C(21)-H(21C)	102.2(19)
C(8)-C(7)-C(6)	118.21(18)	H(21B)-C(21)-H(21C)	111.8(19)
C(9)-C(8)-C(7)	120.2(2)	C(25)-C(22)-C(24)	107.5(2)

C(25)-C(22)-C(4)	110.18(19)	C(16)-C(30)-C(31)	109.77(17)
C(24)-C(22)-C(4)	112.11(19)	C(32)-C(30)-C(31)	109.77(19)
C(25)-C(22)-C(23)	109.0(2)	C(30)-C(31)-H(31A)	110.2(14)
C(24)-C(22)-C(23)	108.9(2)	C(30)-C(31)-H(31B)	113.0(15)
C(4)-C(22)-C(23)	109.08(19)	H(31A)-C(31)-H(31B)	104(2)
C(22)-C(23)-H(23A)	109.1(16)	C(30)-C(31)-H(31C)	106.7(14)
C(22)-C(23)-H(23B)	108.7(17)	H(31A)-C(31)-H(31C)	111(2)
H(23A)-C(23)-H(23B)	104(2)	H(31B)-C(31)-H(31C)	112(2)
C(22)-C(23)-H(23C)	106.4(16)	C(30)-C(32)-H(32A)	109.8(13)
H(23A)-C(23)-H(23C)	118(2)	C(30)-C(32)-H(32B)	115.3(15)
H(23B)-C(23)-H(23C)	111(2)	H(32A)-C(32)-H(32B)	107.2(19)
C(22)-C(24)-H(24A)	104.9(16)	C(30)-C(32)-H(32C)	112.8(14)
C(22)-C(24)-H(24B)	103(2)	H(32A)-C(32)-H(32C)	110.5(19)
H(24A)-C(24)-H(24B)	108(3)	H(32B)-C(32)-H(32C)	101(2)
C(22)-C(24)-H(24C)	102.8(16)	C(30)-C(33)-H(33A)	110.8(14)
H(24A)-C(24)-H(24C)	116(2)	C(30)-C(33)-H(33B)	106.0(14)
H(24B)-C(24)-H(24C)	120(3)	H(33A)-C(33)-H(33B)	111.9(19)
C(22)-C(25)-H(25A)	108.2(16)	C(30)-C(33)-H(33C)	108.3(15)
C(22)-C(25)-H(25B)	108.6(16)	H(33A)-C(33)-H(33C)	104.8(18)
H(25A)-C(25)-H(25B)	104(2)	H(33B)-C(33)-H(33C)	115(2)
C(22)-C(25)-H(25C)	107.2(17)	N(2)-C(34)-H(34A)	103.6(13)
H(25A)-C(25)-H(25C)	117(2)	N(2)-C(34)-H(34B)	106.5(18)
H(25B)-C(25)-H(25C)	112(2)	H(34A)-C(34)-H(34B)	114(2)
C(29)-C(26)-C(27)	107.9(2)	N(2)-C(34)-H(34C)	107.6(18)
C(29)-C(26)-C(28)	109.3(2)	H(34A)-C(34)-H(34C)	112(2)
C(27)-C(26)-C(28)	109.0(2)	H(34B)-C(34)-H(34C)	113(2)
C(29)-C(26)-C(14)	111.48(19)	N(2)-C(35)-H(35A)	112.0(13)
C(27)-C(26)-C(14)	109.34(17)	N(2)-C(35)-H(35B)	110.2(15)
C(28)-C(26)-C(14)	109.81(19)	H(35A)-C(35)-H(35B)	107.2(19)
C(26)-C(27)-H(27A)	106.2(15)	N(2)-C(35)-H(35C)	106.8(15)
C(26)-C(27)-H(27B)	111.2(15)	H(35A)-C(35)-H(35C)	107(2)
H(27A)-C(27)-H(27B)	111(2)	H(35B)-C(35)-H(35C)	113(2)
C(26)-C(27)-H(27C)	105.5(17)	N(3)-C(36)-C(37)	120.4(2)
H(27A)-C(27)-H(27C)	112(2)	N(3)-C(36)-C(41)	121.30(19)
H(27B)-C(27)-H(27C)	111(2)	C(37)-C(36)-C(41)	118.3(2)
C(26)-C(28)-H(28A)	113.5(14)	C(36)-C(37)-C(38)	119.9(2)
C(26)-C(28)-H(28B)	106(2)	C(36)-C(37)-H(37)	117.2(14)
H(28A)-C(28)-H(28B)	115(2)	C(38)-C(37)-H(37)	122.6(14)
C(26)-C(28)-H(28C)	109.3(16)	C(39)-C(38)-C(37)	120.8(3)
H(28A)-C(28)-H(28C)	106(2)	C(39)-C(38)-H(38)	119.3(18)
H(28B)-C(28)-H(28C)	107(2)	C(37)-C(38)-H(38)	119.7(18)
C(26)-C(29)-H(29A)	107.2(17)	C(38)-C(39)-C(40)	120.2(2)
C(26)-C(29)-H(29B)	109.3(17)	C(38)-C(39)-H(39)	122.1(17)
H(29A)-C(29)-H(29B)	111(2)	C(40)-C(39)-H(39)	117.7(17)
C(26)-C(29)-H(29C)	105.6(12)	C(39)-C(40)-C(41)	119.9(2)
H(29A)-C(29)-H(29C)	106.8(19)	C(39)-C(40)-H(40)	122.6(14)
H(29B)-C(29)-H(29C)	117(2)	C(41)-C(40)-H(40)	117.5(14)
C(33)-C(30)-C(16)	112.48(17)	C(40)-C(41)-C(36)	120.8(2)
C(33)-C(30)-C(32)	107.20(18)	C(40)-C(41)-H(41)	123.1(15)
C(16)-C(30)-C(32)	110.35(18)	C(36)-C(41)-H(41)	115.9(15)
C(33)-C(30)-C(31)	107.18(19)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT16 (CCDC 694413). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	92(1)	160(1)	121(1)	-38(1)	-6(1)	-13(1)
Cl(1)	117(2)	321(3)	217(3)	-84(2)	-34(2)	-10(2)
O(1)	121(7)	202(7)	118(7)	-31(6)	-36(6)	-3(5)
O(2)	110(7)	148(6)	116(7)	-24(5)	-18(5)	10(5)
N(1)	102(8)	116(7)	107(8)	-13(6)	-12(6)	0(6)
N(2)	177(9)	185(9)	193(10)	-10(7)	-10(8)	1(7)
N(3)	124(8)	164(8)	170(9)	-30(7)	-20(7)	-43(6)
C(1)	148(10)	110(8)	125(10)	-8(7)	-5(8)	-20(7)
C(2)	136(10)	135(9)	150(11)	-21(8)	4(8)	-16(7)
C(3)	194(11)	163(9)	121(11)	-24(8)	45(9)	-26(8)
C(4)	166(10)	156(9)	139(10)	-27(8)	-8(8)	-22(8)
C(5)	114(10)	179(10)	182(11)	-37(8)	-10(9)	-30(8)
C(6)	143(10)	115(8)	126(10)	-28(7)	8(8)	-18(7)
C(7)	129(10)	137(9)	99(10)	-6(7)	-15(8)	10(7)
C(8)	153(10)	150(9)	130(11)	-36(8)	-11(8)	-23(8)
C(9)	115(10)	197(10)	163(11)	-14(8)	-15(8)	-45(8)
C(10)	105(9)	195(10)	141(11)	-19(8)	13(8)	-11(8)
C(11)	112(9)	142(9)	104(10)	-2(7)	-9(8)	-10(7)
C(12)	125(9)	136(9)	106(10)	-10(7)	32(8)	-30(7)
C(13)	116(10)	177(9)	123(10)	11(8)	-2(8)	-23(8)
C(14)	166(10)	140(9)	140(10)	2(8)	38(8)	-2(8)
C(15)	192(11)	145(9)	151(11)	-46(8)	35(9)	-35(8)
C(16)	153(10)	153(9)	120(10)	-14(8)	23(8)	-54(8)
C(17)	114(9)	131(9)	114(10)	12(7)	32(8)	-19(7)
C(18)	124(10)	217(10)	167(11)	-37(8)	3(8)	-20(8)
C(19)	139(11)	205(11)	267(14)	-68(10)	-19(10)	11(9)
C(20)	162(12)	439(16)	226(14)	-85(12)	15(10)	-14(11)
C(21)	152(12)	258(12)	259(14)	9(10)	-13(10)	-69(9)
C(22)	190(11)	283(11)	166(11)	-82(9)	-2(9)	-48(9)
C(23)	493(19)	378(15)	337(17)	-190(13)	-54(15)	-70(14)
C(24)	269(15)	800(20)	246(16)	-239(16)	-38(12)	-63(15)
C(25)	372(17)	495(18)	216(15)	0(13)	-67(12)	-77(14)
C(26)	182(11)	180(10)	208(12)	-55(8)	-6(9)	36(8)
C(27)	240(14)	351(14)	306(16)	-77(12)	16(12)	93(11)
C(28)	378(17)	194(12)	520(20)	17(12)	41(15)	54(11)
C(29)	290(15)	333(14)	385(18)	-135(13)	-96(13)	162(12)
C(30)	156(10)	175(9)	165(11)	-52(8)	-4(8)	-29(8)
C(31)	270(13)	259(12)	170(12)	-46(10)	-75(10)	-43(10)
C(32)	176(12)	304(13)	247(13)	-105(11)	24(10)	-91(10)
C(33)	215(13)	278(13)	266(14)	-120(11)	-51(11)	-14(10)
C(34)	490(20)	185(12)	590(20)	26(13)	198(17)	49(12)
C(35)	239(13)	300(13)	342(16)	71(12)	-20(12)	-75(11)
C(36)	215(11)	194(10)	154(11)	-40(8)	-4(9)	-76(9)
C(37)	350(15)	266(12)	339(15)	-107(11)	160(12)	-106(11)
C(38)	600(20)	290(13)	361(17)	-91(12)	240(15)	-254(13)
C(39)	610(20)	164(11)	299(15)	-16(10)	38(13)	-114(12)
C(40)	352(15)	178(11)	350(15)	-27(10)	-14(12)	-20(10)

C(41)	226(12)	244(11)	248(13)	-14(10)	16(10)	-70(10)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT16 (CCDC 694413).

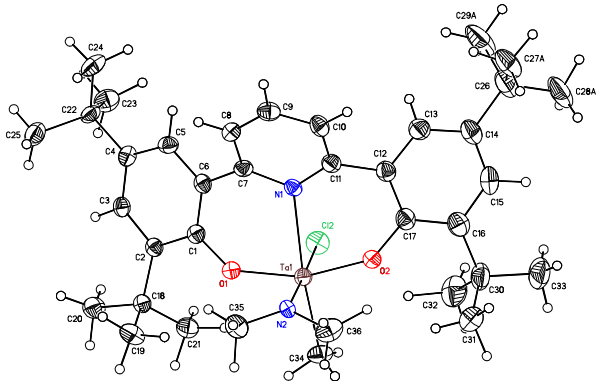
	x	y	z	U_{iso}
H(2)	6820(20)	7850(20)	6013(13)	34(7)
H(3)	6350(20)	7425(19)	10112(12)	21(6)
H(5)	9890(20)	6895(18)	9295(11)	11(5)
H(8)	10735(19)	7650(17)	8310(10)	5(5)
H(9)	12370(20)	7090(19)	7514(11)	17(6)
H(10)	12060(20)	5601(18)	6832(11)	10(5)
H(13)	11940(20)	3381(18)	7029(11)	12(5)
H(15)	10027(18)	1829(17)	5613(10)	4(5)
H(19A)	3200(20)	8450(20)	8429(12)	33(7)
H(19B)	4490(20)	8051(19)	7937(12)	17(6)
H(19C)	4320(30)	9030(20)	8462(14)	40(8)
H(20A)	4180(20)	6997(19)	10083(11)	14(6)
H(20B)	3030(30)	7670(20)	9541(13)	35(7)
H(20C)	4090(20)	8410(20)	9783(12)	21(6)
H(21A)	4560(20)	5400(20)	9265(13)	27(7)
H(21B)	4720(20)	5719(18)	8465(11)	11(5)
H(21C)	3430(20)	6000(20)	8892(12)	26(7)
H(23A)	8720(30)	9360(20)	10324(15)	46(8)
H(23B)	8750(30)	8880(30)	11133(17)	65(10)
H(23C)	7350(30)	8840(20)	10721(14)	50(9)
H(24A)	10640(30)	6230(30)	10481(15)	52(9)
H(24B)	10570(30)	7160(30)	11013(17)	70(11)
H(24C)	10630(30)	7890(30)	10160(16)	68(10)
H(25A)	7370(30)	6660(30)	11204(15)	54(9)
H(25B)	8720(30)	6590(30)	11623(15)	57(9)
H(25C)	8680(30)	5570(30)	11067(16)	64(10)
H(27A)	13460(30)	2140(20)	5537(13)	46(8)
H(27B)	12410(20)	1250(20)	5301(13)	32(7)
H(27C)	13660(30)	620(20)	5692(13)	41(8)
H(28A)	11110(30)	-170(20)	6243(15)	57(9)
H(28B)	11600(30)	-10(30)	7063(17)	64(11)
H(28C)	12590(30)	-690(20)	6602(14)	48(8)
H(29A)	14130(30)	720(20)	6916(13)	38(7)
H(29B)	13120(30)	1400(20)	7357(14)	36(8)
H(29C)	13910(20)	2200(20)	6692(11)	20(6)
H(31A)	8280(30)	4860(20)	4570(13)	39(8)
H(31B)	7290(20)	5350(20)	5056(12)	21(6)
H(31C)	6760(20)	4630(20)	4545(13)	27(7)
H(32A)	5690(20)	3190(20)	5490(12)	30(7)
H(32B)	6260(20)	3760(20)	6069(12)	19(6)
H(32C)	6640(20)	2460(20)	6160(12)	28(7)
H(33A)	8760(20)	2413(19)	4614(12)	22(6)
H(33B)	7220(20)	2424(19)	4639(12)	19(6)
H(33C)	8170(20)	1610(20)	5189(12)	18(6)
H(34A)	7110(20)	9200(20)	7094(13)	30(7)
H(34B)	5610(30)	8780(30)	6803(17)	72(11)
H(34C)	6430(30)	9670(30)	6293(15)	49(9)
H(35A)	8640(20)	8960(20)	5866(12)	26(6)

H(35B)	9160(30)	7440(20)	5991(14)	46(8)
H(35C)	9080(30)	8310(20)	6630(14)	37(8)
H(37)	5240(20)	3130(20)	8349(13)	37(7)
H(38)	5550(30)	960(20)	8924(15)	51(9)
H(39)	7370(20)	-410(20)	8711(12)	30(7)
H(40)	8970(20)	200(20)	7961(11)	17(6)
H(41)	8730(20)	2270(20)	7444(12)	20(6)

Crystal Structure Analysis of:

Complex 6 (IAT21)

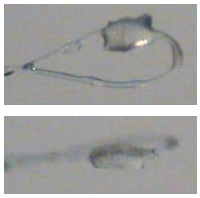
Contents



IAT21

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 698486. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 698486."

Table 1. Crystal data and structure refinement for IAT21 (CCDC 698486).



Empirical formula	$C_{36}H_{52}N_2O_2ClTa \bullet C_4H_{10}O$
Formula weight	835.32
Crystallization Solvent	Diethylether
Crystal Habit	Flake
Crystal size	0.22 x 0.13 x 0.04 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9924 reflections used in lattice determination	2.32 to 27.32°
Unit cell dimensions	a = 47.432(2) Å b = 13.7447(7) Å β= 100.510(3)° c = 12.4876(6) Å
Volume	8004.5(7) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	C2/*c*
Density (calculated)	1.386 Mg/m^3
F(000)	3440
θ range for data collection	1.54 to 27.85°
Completeness to θ = 27.85°	90.1 %
Index ranges	$-60 \le h \le 60$, $-17 \le k \le 17$, $-16 \le l \le 16$
Data collection scan type	ω scans; 11 settings
Reflections collected	63460
Independent reflections	8588 [R_{int}= 0.0730]
Absorption coefficient	2.850 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8945 and 0.5729

Table 1 (cont.)

Structure solution and Refinement

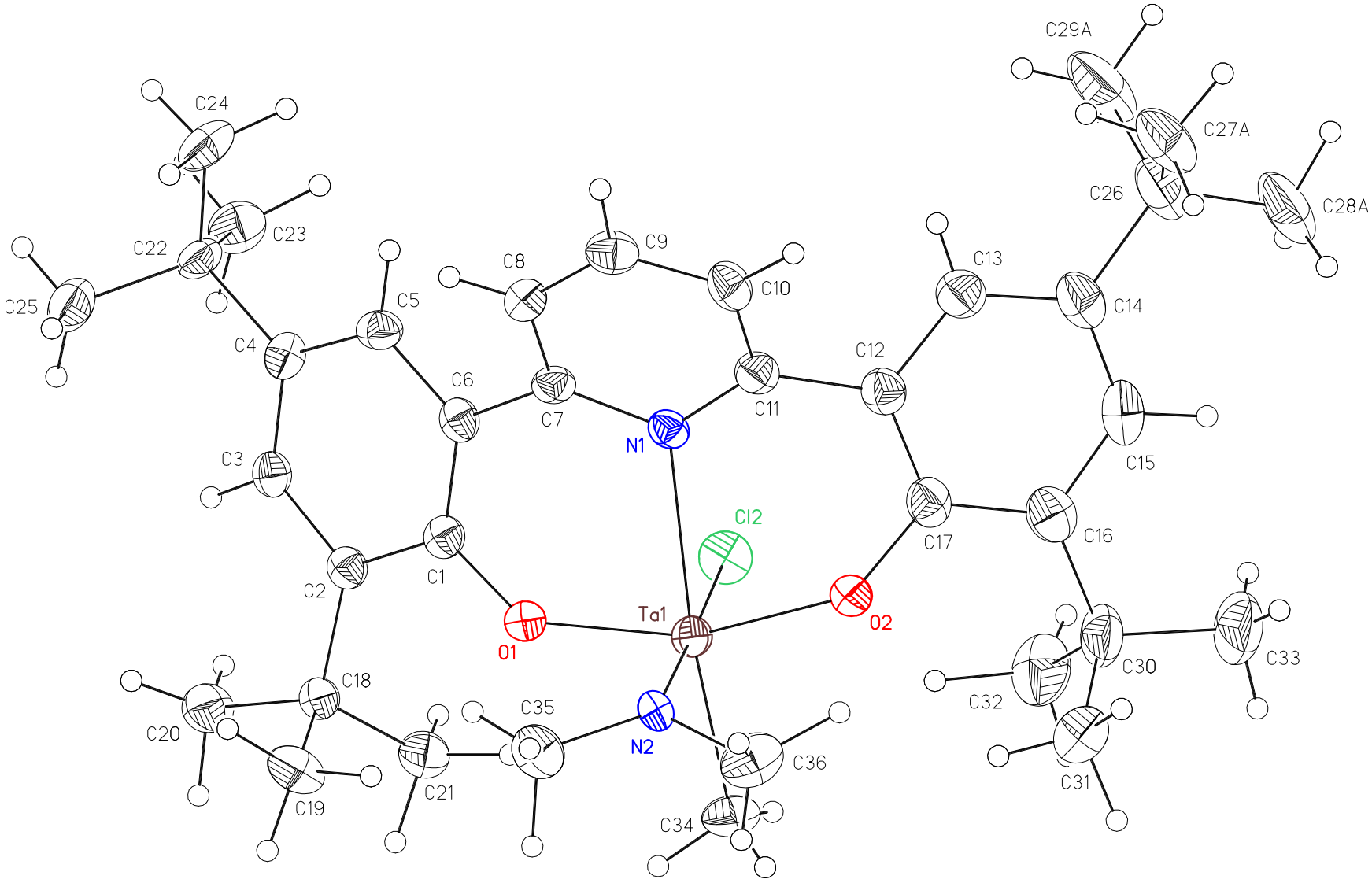
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	8588 / 0 / 632
Treatment of hydrogen atoms	Mixed
Goodness-of-fit on F^2	1.678
Final R indices [$I>2\sigma(I)$, 6077 reflections]	R1 = 0.0358, *w*R2 = 0.0563
R indices (all data)	R1 = 0.0623, *w*R2 = 0.0577
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	2.305 and -1.993 e.Å^{-3}

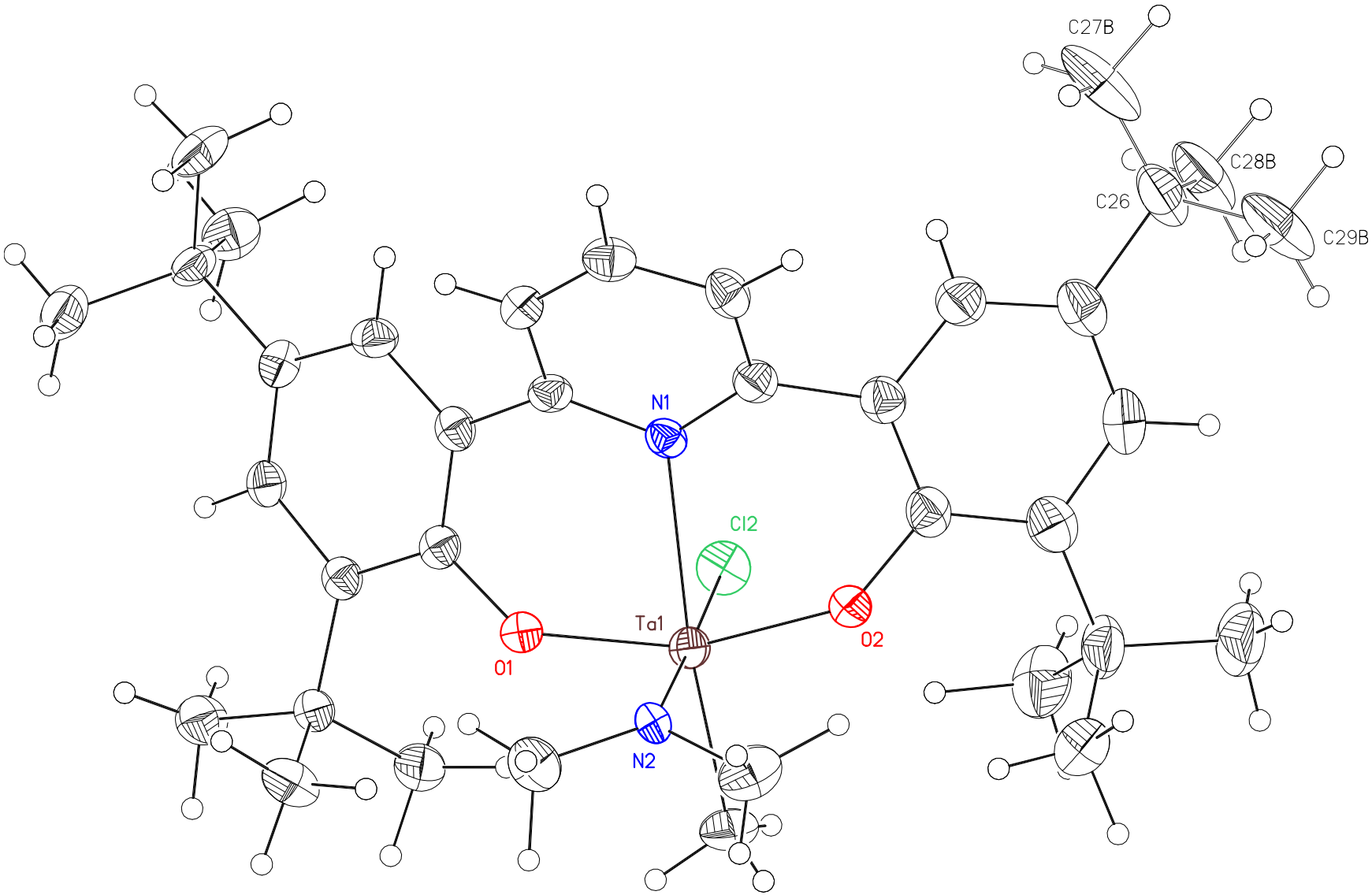
Special Refinement Details

Crystals were mounted on a loop using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C29A
C24
C27A
C26
C28A
C22
C23
C13
C25
C5
C8
C9
C10
C14
C4
C12
C6
C7
C11
N1
C3
C15
Cl2
C17
C16
C2
C1
Ta1
O2
O1
C18
C30
C33
C32
C35
C20
N2
C36
C19
C21
C31
C34


C27B
C28B
C26
C29B
N1
Cl2
Ta1
O1
O2
N2

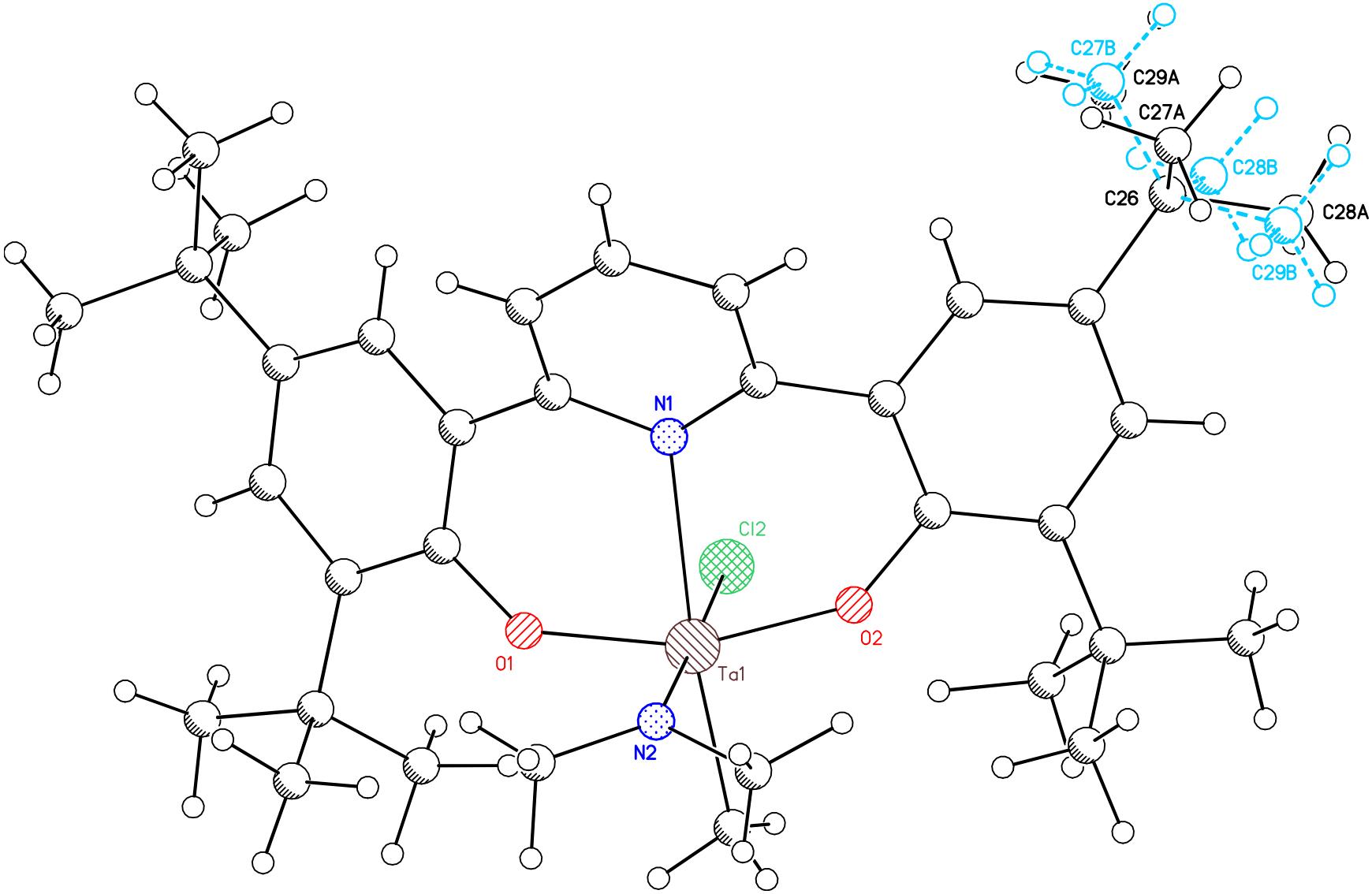

C27B
C29A
C27A
C28B
C26
C28A
C29B
N1
Cl2
O1
O2
Ta1
N2

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT21 (CCDC 698486). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ta(1)	3421(1)	7288(1)	2319(1)	23(1)	1
Cl(2)	3683(1)	8069(1)	1016(1)	34(1)	1
O(1)	3157(1)	8332(2)	2051(2)	25(1)	1
O(2)	3754(1)	6578(2)	2877(2)	26(1)	1
N(1)	3674(1)	8445(2)	3567(3)	20(1)	1
N(2)	3180(1)	6665(2)	3258(3)	25(1)	1
C(1)	3154(1)	9327(3)	2052(3)	22(1)	1
C(2)	2963(1)	9859(3)	1263(3)	22(1)	1
C(3)	2985(1)	10873(3)	1316(3)	23(1)	1
C(4)	3174(1)	11374(3)	2109(3)	25(1)	1
C(5)	3352(1)	10823(3)	2894(3)	25(1)	1
C(6)	3342(1)	9796(3)	2883(3)	22(1)	1
C(7)	3530(1)	9275(3)	3773(3)	22(1)	1
C(8)	3574(1)	9681(3)	4807(4)	26(1)	1
C(9)	3773(1)	9306(3)	5632(4)	29(1)	1
C(10)	3942(1)	8546(3)	5397(4)	29(1)	1
C(11)	3894(1)	8134(3)	4352(3)	25(1)	1
C(12)	4106(1)	7442(3)	4084(3)	28(1)	1
C(13)	4391(1)	7569(3)	4566(4)	32(1)	1
C(14)	4611(1)	6986(3)	4322(4)	36(1)	1
C(15)	4531(1)	6227(4)	3579(4)	40(1)	1
C(16)	4250(1)	6054(3)	3063(4)	35(1)	1
C(17)	4034(1)	6681(3)	3334(3)	29(1)	1
C(18)	2729(1)	9364(3)	419(3)	25(1)	1
C(19)	2533(1)	8798(4)	1039(4)	37(1)	1
C(20)	2545(1)	10098(4)	-309(4)	34(1)	1
C(21)	2859(1)	8671(4)	-311(4)	35(1)	1
C(22)	3186(1)	12489(3)	2091(3)	26(1)	1
C(23)	3353(1)	12792(4)	1205(4)	38(1)	1
C(24)	3339(1)	12892(4)	3184(4)	38(1)	1
C(25)	2885(1)	12902(4)	1850(5)	37(1)	1
C(26)	4923(1)	7184(4)	4839(4)	46(1)	1
C(27A)	4953(1)	7089(6)	6108(6)	49(3)	0.672(9)
C(28A)	5138(2)	6522(7)	4477(9)	70(4)	0.672(9)
C(29A)	5003(2)	8258(7)	4628(8)	68(3)	0.672(9)
C(27B)	4966(3)	8020(14)	5608(16)	72(7)	0.328(9)
C(28B)	5078(3)	7410(13)	3845(14)	59(6)	0.328(9)
C(29B)	5053(3)	6221(13)	5355(16)	65(7)	0.328(9)
C(30)	4174(1)	5220(3)	2233(4)	42(1)	1
C(31)	3949(1)	4541(4)	2562(5)	49(2)	1
C(32)	4061(1)	5651(5)	1093(5)	52(2)	1
C(33)	4440(1)	4600(5)	2144(6)	58(2)	1
C(34)	3246(1)	6252(4)	1034(4)	34(1)	1
C(35)	2889(1)	6953(4)	3364(4)	34(1)	1
C(36)	3247(1)	5684(4)	3725(5)	40(1)	1

O(40)	4328(1)	9291(3)	7784(3)	62(1)	1
C(41)	4515(2)	10506(7)	6860(7)	252(8)	1
C(42)	4370(2)	10313(5)	7781(7)	125(3)	1
C(43)	4208(1)	9036(5)	8700(5)	77(2)	1
C(44)	4145(1)	7982(5)	8659(5)	90(2)	1

Table 3. Selected bond lengths [Å] and angles [°] for IAT21 (CCDC 698486).

Ta(1)-O(2)	1.881(3)	O(2)-Ta(1)-O(1)	160.50(11)
Ta(1)-O(1)	1.894(3)	O(2)-Ta(1)-N(2)	95.39(12)
Ta(1)-N(2)	1.974(3)	O(1)-Ta(1)-N(2)	89.89(12)
Ta(1)-C(34)	2.191(5)	O(2)-Ta(1)-C(34)	96.53(17)
Ta(1)-N(1)	2.392(3)	O(1)-Ta(1)-C(34)	102.38(17)
Ta(1)-Cl(2)	2.4681(11)	N(2)-Ta(1)-C(34)	88.38(18)
		O(2)-Ta(1)-N(1)	79.32(11)
		O(1)-Ta(1)-N(1)	81.28(11)
		N(2)-Ta(1)-N(1)	100.21(12)
		C(34)-Ta(1)-N(1)	170.73(18)
		O(2)-Ta(1)-Cl(2)	88.75(8)
		O(1)-Ta(1)-Cl(2)	87.17(8)
		N(2)-Ta(1)-Cl(2)	174.89(10)
		C(34)-Ta(1)-Cl(2)	88.17(16)
		N(1)-Ta(1)-Cl(2)	83.48(8)

Table 4. Bond lengths [Å] and angles [°] for IAT21 (CCDC 698486).

Ta(1)-O(2)	1.881(3)	C(21)-H(21B)	1.04(4)
Ta(1)-O(1)	1.894(3)	C(21)-H(21C)	0.92(4)
Ta(1)-N(2)	1.974(3)	C(22)-C(25)	1.518(6)
Ta(1)-C(34)	2.191(5)	C(22)-C(24)	1.527(6)
Ta(1)-N(1)	2.392(3)	C(22)-C(23)	1.529(6)
Ta(1)-Cl(2)	2.4681(11)	C(23)-H(23A)	1.01(4)
O(1)-C(1)	1.368(4)	C(23)-H(23B)	1.03(4)
O(2)-C(17)	1.354(5)	C(23)-H(23C)	1.01(4)
N(1)-C(11)	1.363(5)	C(24)-H(24A)	0.92(4)
N(1)-C(7)	1.377(5)	C(24)-H(24B)	0.98(4)
N(2)-C(35)	1.463(5)	C(24)-H(24C)	1.11(4)
N(2)-C(36)	1.480(6)	C(25)-H(25A)	0.89(4)
C(1)-C(6)	1.397(5)	C(25)-H(25B)	0.98(4)
C(1)-C(2)	1.414(5)	C(25)-H(25C)	1.00(4)
C(2)-C(3)	1.398(5)	C(26)-C(27B)	1.487(19)
C(2)-C(18)	1.543(5)	C(26)-C(28A)	1.496(9)
C(3)-C(4)	1.391(5)	C(26)-C(29B)	1.549(17)
C(3)-H(3)	0.95(4)	C(26)-C(29A)	1.558(9)
C(4)-C(5)	1.394(5)	C(26)-C(27A)	1.570(9)
C(4)-C(22)	1.534(5)	C(26)-C(28B)	1.586(16)
C(5)-C(6)	1.412(5)	C(27A)-H(27A)	0.9800
C(5)-H(5)	0.94(3)	C(27A)-H(27B)	0.9800
C(6)-C(7)	1.478(5)	C(27A)-H(27C)	0.9800
C(7)-C(8)	1.387(5)	C(28A)-H(28A)	0.9800
C(8)-C(9)	1.366(6)	C(28A)-H(28B)	0.9800
C(8)-H(8)	0.89(3)	C(28A)-H(28C)	0.9800
C(9)-C(10)	1.379(6)	C(29A)-H(29A)	0.9800
C(9)-H(9)	1.02(4)	C(29A)-H(29B)	0.9800
C(10)-C(11)	1.402(6)	C(29A)-H(29C)	0.9800
C(10)-H(10)	0.90(3)	C(27B)-H(27D)	0.9800
C(11)-C(12)	1.467(5)	C(27B)-H(27E)	0.9800
C(12)-C(13)	1.389(5)	C(27B)-H(27F)	0.9800
C(12)-C(17)	1.403(5)	C(28B)-H(28D)	0.9800
C(13)-C(14)	1.394(6)	C(28B)-H(28E)	0.9800
C(13)-H(13)	0.84(3)	C(28B)-H(28F)	0.9800
C(14)-C(15)	1.402(6)	C(29B)-H(29D)	0.9800
C(14)-C(26)	1.526(6)	C(29B)-H(29E)	0.9800
C(15)-C(16)	1.389(6)	C(29B)-H(29F)	0.9800
C(15)-H(15)	0.97(4)	C(30)-C(31)	1.530(7)
C(16)-C(17)	1.425(6)	C(30)-C(32)	1.545(7)
C(16)-C(30)	1.543(6)	C(30)-C(33)	1.544(7)
C(18)-C(20)	1.522(6)	C(31)-H(31A)	1.01(5)
C(18)-C(21)	1.526(6)	C(31)-H(31B)	1.09(5)
C(18)-C(19)	1.529(6)	C(31)-H(31C)	0.97(5)
C(19)-H(19A)	1.03(4)	C(32)-H(32A)	1.19(5)
C(19)-H(19B)	1.05(4)	C(32)-H(32B)	1.05(5)
C(19)-H(19C)	0.98(4)	C(32)-H(32C)	0.96(5)
C(20)-H(20A)	1.01(4)	C(33)-H(33A)	1.02(5)
C(20)-H(20B)	0.90(4)	C(33)-H(33B)	0.98(5)
C(20)-H(20C)	1.03(4)	C(33)-H(33C)	1.02(5)
C(21)-H(21A)	1.06(4)	C(34)-H(34A)	0.87(5)

C(34)-H(34B)	1.03(5)	C(2)-C(3)-H(3)	114(2)
C(34)-H(34C)	0.95(6)	C(3)-C(4)-C(5)	117.4(4)
C(35)-H(35A)	1.07(5)	C(3)-C(4)-C(22)	120.4(4)
C(35)-H(35B)	0.98(4)	C(5)-C(4)-C(22)	122.2(4)
C(35)-H(35C)	1.02(4)	C(4)-C(5)-C(6)	121.5(4)
C(36)-H(36A)	0.95(4)	C(4)-C(5)-H(5)	119(2)
C(36)-H(36B)	1.12(4)	C(6)-C(5)-H(5)	120(2)
C(36)-H(36C)	0.90(4)	C(1)-C(6)-C(5)	118.9(4)
O(40)-C(43)	1.413(7)	C(1)-C(6)-C(7)	123.5(4)
O(40)-C(42)	1.418(6)	C(5)-C(6)-C(7)	117.6(4)
C(41)-C(42)	1.467(11)	N(1)-C(7)-C(8)	120.8(4)
C(41)-H(41A)	0.9800	N(1)-C(7)-C(6)	120.8(4)
C(41)-H(41B)	0.9800	C(8)-C(7)-C(6)	118.3(4)
C(41)-H(41C)	0.9800	C(9)-C(8)-C(7)	121.1(4)
C(42)-H(42A)	0.9900	C(9)-C(8)-H(8)	122(2)
C(42)-H(42B)	0.9900	C(7)-C(8)-H(8)	117(2)
C(43)-C(44)	1.478(7)	C(8)-C(9)-C(10)	118.2(4)
C(43)-H(43A)	0.9900	C(8)-C(9)-H(9)	127(2)
C(43)-H(43B)	0.9900	C(10)-C(9)-H(9)	115(2)
C(44)-H(44A)	0.9800	C(9)-C(10)-C(11)	120.2(4)
C(44)-H(44B)	0.9800	C(9)-C(10)-H(10)	124(2)
C(44)-H(44C)	0.9800	C(11)-C(10)-H(10)	116(2)
		N(1)-C(11)-C(10)	121.1(4)
O(2)-Ta(1)-O(1)	160.50(11)	N(1)-C(11)-C(12)	120.4(4)
O(2)-Ta(1)-N(2)	95.39(12)	C(10)-C(11)-C(12)	118.2(4)
O(1)-Ta(1)-N(2)	89.89(12)	C(13)-C(12)-C(17)	118.7(4)
O(2)-Ta(1)-C(34)	96.53(17)	C(13)-C(12)-C(11)	118.3(4)
O(1)-Ta(1)-C(34)	102.38(17)	C(17)-C(12)-C(11)	122.9(4)
N(2)-Ta(1)-C(34)	88.38(18)	C(12)-C(13)-C(14)	122.9(4)
O(2)-Ta(1)-N(1)	79.32(11)	C(12)-C(13)-H(13)	123(3)
O(1)-Ta(1)-N(1)	81.28(11)	C(14)-C(13)-H(13)	114(3)
N(2)-Ta(1)-N(1)	100.21(12)	C(13)-C(14)-C(15)	116.5(4)
C(34)-Ta(1)-N(1)	170.73(18)	C(13)-C(14)-C(26)	120.8(4)
O(2)-Ta(1)-Cl(2)	88.75(8)	C(15)-C(14)-C(26)	122.7(4)
O(1)-Ta(1)-Cl(2)	87.17(8)	C(16)-C(15)-C(14)	123.9(4)
N(2)-Ta(1)-Cl(2)	174.89(10)	C(16)-C(15)-H(15)	120(3)
C(34)-Ta(1)-Cl(2)	88.17(16)	C(14)-C(15)-H(15)	116(3)
N(1)-Ta(1)-Cl(2)	83.48(8)	C(15)-C(16)-C(17)	117.0(4)
C(1)-O(1)-Ta(1)	139.8(2)	C(15)-C(16)-C(30)	121.7(4)
C(17)-O(2)-Ta(1)	142.8(3)	C(17)-C(16)-C(30)	121.3(4)
C(11)-N(1)-C(7)	117.7(3)	O(2)-C(17)-C(12)	117.2(4)
C(11)-N(1)-Ta(1)	119.2(3)	O(2)-C(17)-C(16)	121.9(4)
C(7)-N(1)-Ta(1)	117.8(2)	C(12)-C(17)-C(16)	120.8(4)
C(35)-N(2)-C(36)	110.4(4)	C(20)-C(18)-C(21)	107.9(4)
C(35)-N(2)-Ta(1)	126.3(3)	C(20)-C(18)-C(19)	107.7(4)
C(36)-N(2)-Ta(1)	121.5(3)	C(21)-C(18)-C(19)	109.6(4)
O(1)-C(1)-C(6)	117.3(3)	C(20)-C(18)-C(2)	112.3(3)
O(1)-C(1)-C(2)	121.4(3)	C(21)-C(18)-C(2)	111.4(4)
C(6)-C(1)-C(2)	121.3(4)	C(19)-C(18)-C(2)	107.9(4)
C(3)-C(2)-C(1)	116.7(4)	C(18)-C(19)-H(19A)	109(2)
C(3)-C(2)-C(18)	120.6(3)	C(18)-C(19)-H(19B)	114(3)
C(1)-C(2)-C(18)	122.5(4)	H(19A)-C(19)-H(19B)	108(3)
C(4)-C(3)-C(2)	124.1(4)	C(18)-C(19)-H(19C)	111(3)
C(4)-C(3)-H(3)	121(2)	H(19A)-C(19)-H(19C)	106(3)

H(19B)-C(19)-H(19C)	109(3)	C(14)-C(26)-C(28B)	104.8(6)
C(18)-C(20)-H(20A)	108(2)	C(29B)-C(26)-C(28B)	106.7(10)
C(18)-C(20)-H(20B)	106(2)	C(29A)-C(26)-C(28B)	61.3(7)
H(20A)-C(20)-H(20B)	108(3)	C(27A)-C(26)-C(28B)	146.8(7)
C(18)-C(20)-H(20C)	112(2)	C(26)-C(27A)-H(27A)	109.5
H(20A)-C(20)-H(20C)	109(3)	C(26)-C(27A)-H(27B)	109.5
H(20B)-C(20)-H(20C)	114(4)	C(26)-C(27A)-H(27C)	109.5
C(18)-C(21)-H(21A)	106(2)	C(26)-C(28A)-H(28A)	109.5
C(18)-C(21)-H(21B)	121(2)	C(26)-C(28A)-H(28B)	109.5
H(21A)-C(21)-H(21B)	112(3)	C(26)-C(28A)-H(28C)	109.5
C(18)-C(21)-H(21C)	111(3)	C(26)-C(29A)-H(29A)	109.5
H(21A)-C(21)-H(21C)	106(4)	C(26)-C(29A)-H(29B)	109.5
H(21B)-C(21)-H(21C)	100(4)	C(26)-C(29A)-H(29C)	109.5
C(25)-C(22)-C(24)	108.6(4)	C(26)-C(27B)-H(27D)	109.5
C(25)-C(22)-C(23)	110.4(4)	C(26)-C(27B)-H(27E)	109.5
C(24)-C(22)-C(23)	108.9(4)	H(27D)-C(27B)-H(27E)	109.5
C(25)-C(22)-C(4)	109.8(4)	C(26)-C(27B)-H(27F)	109.5
C(24)-C(22)-C(4)	111.2(3)	H(27D)-C(27B)-H(27F)	109.5
C(23)-C(22)-C(4)	108.0(3)	H(27E)-C(27B)-H(27F)	109.5
C(22)-C(23)-H(23A)	103(2)	C(26)-C(28B)-H(28D)	109.5
C(22)-C(23)-H(23B)	110(2)	C(26)-C(28B)-H(28E)	109.5
H(23A)-C(23)-H(23B)	126(3)	H(28D)-C(28B)-H(28E)	109.5
C(22)-C(23)-H(23C)	112(2)	C(26)-C(28B)-H(28F)	109.5
H(23A)-C(23)-H(23C)	105(3)	H(28D)-C(28B)-H(28F)	109.5
H(23B)-C(23)-H(23C)	102(3)	H(28E)-C(28B)-H(28F)	109.5
C(22)-C(24)-H(24A)	109(2)	C(26)-C(29B)-H(29D)	109.5
C(22)-C(24)-H(24B)	112(2)	C(26)-C(29B)-H(29E)	109.5
H(24A)-C(24)-H(24B)	108(3)	H(29D)-C(29B)-H(29E)	109.5
C(22)-C(24)-H(24C)	104(2)	C(26)-C(29B)-H(29F)	109.5
H(24A)-C(24)-H(24C)	106(3)	H(29D)-C(29B)-H(29F)	109.5
H(24B)-C(24)-H(24C)	118(3)	H(29E)-C(29B)-H(29F)	109.5
C(22)-C(25)-H(25A)	109(3)	C(31)-C(30)-C(16)	111.2(4)
C(22)-C(25)-H(25B)	108(2)	C(31)-C(30)-C(32)	109.9(5)
H(25A)-C(25)-H(25B)	111(4)	C(16)-C(30)-C(32)	109.5(4)
C(22)-C(25)-H(25C)	115(2)	C(31)-C(30)-C(33)	107.6(5)
H(25A)-C(25)-H(25C)	107(4)	C(16)-C(30)-C(33)	111.4(4)
H(25B)-C(25)-H(25C)	107(3)	C(32)-C(30)-C(33)	107.2(5)
C(27B)-C(26)-C(28A)	130.2(8)	C(30)-C(31)-H(31A)	108(3)
C(27B)-C(26)-C(14)	114.6(7)	C(30)-C(31)-H(31B)	112(3)
C(28A)-C(26)-C(14)	115.1(5)	H(31A)-C(31)-H(31B)	110(4)
C(27B)-C(26)-C(29B)	113.3(10)	C(30)-C(31)-H(31C)	117(3)
C(28A)-C(26)-C(29B)	50.6(7)	H(31A)-C(31)-H(31C)	110(4)
C(14)-C(26)-C(29B)	107.8(7)	H(31B)-C(31)-H(31C)	101(4)
C(27B)-C(26)-C(29A)	50.8(8)	C(30)-C(32)-H(32A)	112(2)
C(28A)-C(26)-C(29A)	109.0(6)	C(30)-C(32)-H(32B)	112(3)
C(14)-C(26)-C(29A)	110.0(4)	H(32A)-C(32)-H(32B)	102(4)
C(29B)-C(26)-C(29A)	142.1(7)	C(30)-C(32)-H(32C)	109(3)
C(27B)-C(26)-C(27A)	55.7(8)	H(32A)-C(32)-H(32C)	115(4)
C(28A)-C(26)-C(27A)	108.3(6)	H(32B)-C(32)-H(32C)	106(4)
C(14)-C(26)-C(27A)	108.4(4)	C(30)-C(33)-H(33A)	106(3)
C(29B)-C(26)-C(27A)	63.5(8)	C(30)-C(33)-H(33B)	103(3)
C(29A)-C(26)-C(27A)	105.6(6)	H(33A)-C(33)-H(33B)	104(5)
C(27B)-C(26)-C(28B)	109.0(10)	C(30)-C(33)-H(33C)	108(3)
C(28A)-C(26)-C(28B)	56.2(7)	H(33A)-C(33)-H(33C)	122(4)

H(33B)-C(33)-H(33C)	113(4)	H(41A)-C(41)-H(41B)	109.5
Ta(1)-C(34)-H(34A)	111(3)	C(42)-C(41)-H(41C)	109.5
Ta(1)-C(34)-H(34B)	116(3)	H(41A)-C(41)-H(41C)	109.5
H(34A)-C(34)-H(34B)	103(4)	H(41B)-C(41)-H(41C)	109.5
Ta(1)-C(34)-H(34C)	113(4)	O(40)-C(42)-C(41)	105.5(7)
H(34A)-C(34)-H(34C)	114(5)	O(40)-C(42)-H(42A)	110.6
H(34B)-C(34)-H(34C)	100(4)	C(41)-C(42)-H(42A)	110.6
N(2)-C(35)-H(35A)	108(2)	O(40)-C(42)-H(42B)	110.6
N(2)-C(35)-H(35B)	112(2)	C(41)-C(42)-H(42B)	110.6
H(35A)-C(35)-H(35B)	108(3)	H(42A)-C(42)-H(42B)	108.8
N(2)-C(35)-H(35C)	113(2)	O(40)-C(43)-C(44)	108.9(5)
H(35A)-C(35)-H(35C)	102(3)	O(40)-C(43)-H(43A)	109.9
H(35B)-C(35)-H(35C)	114(3)	C(44)-C(43)-H(43A)	109.9
N(2)-C(36)-H(36A)	112(2)	O(40)-C(43)-H(43B)	109.9
N(2)-C(36)-H(36B)	112.6(18)	C(44)-C(43)-H(43B)	109.9
H(36A)-C(36)-H(36B)	99(3)	H(43A)-C(43)-H(43B)	108.3
N(2)-C(36)-H(36C)	105(3)	C(43)-C(44)-H(44A)	109.5
H(36A)-C(36)-H(36C)	102(4)	C(43)-C(44)-H(44B)	109.5
H(36B)-C(36)-H(36C)	126(4)	H(44A)-C(44)-H(44B)	109.5
C(43)-O(40)-C(42)	109.0(5)	C(43)-C(44)-H(44C)	109.5
C(42)-C(41)-H(41A)	109.5	H(44A)-C(44)-H(44C)	109.5
C(42)-C(41)-H(41B)	109.5	H(44B)-C(44)-H(44C)	109.5

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT21 (CCDC 698486). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	229(1)	205(1)	235(1)	10(1)	7(1)	9(1)
Cl(2)	361(7)	364(7)	303(6)	27(5)	79(5)	-9(5)
O(1)	227(17)	218(18)	296(17)	-24(13)	16(13)	-3(13)
O(2)	234(17)	231(17)	286(17)	-14(13)	4(14)	7(13)
N(1)	178(19)	210(20)	220(19)	26(15)	33(16)	-22(15)
N(2)	153(19)	240(20)	360(20)	-41(17)	21(16)	18(15)
C(1)	220(20)	240(30)	220(20)	-9(19)	86(19)	1(19)
C(2)	210(20)	250(30)	200(20)	-8(19)	59(19)	9(19)
C(3)	230(30)	230(30)	230(20)	40(20)	40(20)	30(20)
C(4)	290(30)	230(30)	230(20)	5(19)	60(20)	40(20)
C(5)	250(30)	270(30)	240(20)	-50(20)	50(20)	-40(20)
C(6)	200(20)	270(30)	210(20)	-1(19)	68(19)	15(19)
C(7)	220(20)	190(30)	250(20)	15(19)	50(20)	-46(19)
C(8)	260(30)	220(30)	290(30)	-20(20)	40(20)	10(20)
C(9)	320(30)	300(30)	240(30)	10(20)	20(20)	-60(20)
C(10)	250(30)	320(30)	270(30)	60(20)	0(20)	30(20)
C(11)	250(20)	240(30)	270(20)	30(20)	30(20)	-10(20)
C(12)	250(20)	280(30)	300(20)	30(20)	62(19)	0(20)
C(13)	310(30)	300(40)	350(30)	30(20)	40(20)	-10(20)
C(14)	270(30)	410(30)	390(30)	110(20)	30(20)	30(20)
C(15)	340(30)	410(30)	440(30)	70(30)	100(30)	150(30)
C(16)	330(30)	390(30)	310(30)	60(20)	50(20)	30(20)
C(17)	280(30)	270(30)	320(30)	80(20)	40(20)	20(20)
C(18)	230(20)	230(30)	280(20)	0(20)	-10(20)	20(20)
C(19)	280(30)	440(40)	380(30)	20(30)	0(30)	-70(30)
C(20)	360(30)	320(30)	320(30)	30(30)	-30(30)	0(30)
C(21)	320(30)	370(30)	330(30)	-60(30)	-10(30)	10(30)
C(22)	330(20)	150(30)	270(20)	-5(17)	3(19)	0(19)
C(23)	450(30)	310(30)	380(30)	40(30)	80(30)	-40(30)
C(24)	560(40)	180(40)	380(30)	-20(20)	80(30)	-10(30)
C(25)	430(30)	250(40)	440(30)	-10(30)	90(30)	50(30)
C(26)	230(30)	540(40)	590(30)	110(30)	0(20)	40(30)
C(27A)	290(40)	660(80)	480(50)	210(40)	-30(40)	0(40)
C(28A)	210(50)	950(90)	940(90)	-100(70)	60(50)	80(50)
C(29A)	250(50)	840(80)	890(90)	260(60)	-10(50)	-90(50)
C(27B)	200(90)	1200(200)	700(150)	200(140)	-10(90)	-130(100)
C(28B)	210(80)	720(160)	800(130)	330(110)	10(80)	-40(90)
C(29B)	280(100)	910(160)	670(150)	180(120)	-130(100)	-90(100)
C(30)	380(30)	450(30)	440(30)	-70(30)	90(30)	160(30)
C(31)	490(40)	380(40)	580(40)	-90(30)	50(30)	40(30)
C(32)	620(40)	610(40)	360(30)	-60(30)	130(30)	150(40)
C(33)	520(40)	600(50)	650(50)	-140(40)	160(40)	210(40)
C(34)	400(30)	320(30)	290(30)	-70(20)	10(30)	-90(30)
C(35)	310(30)	400(30)	330(30)	50(20)	90(20)	-20(20)
C(36)	560(40)	310(30)	360(30)	70(30)	110(30)	-60(30)

O(40)	790(30)	540(30)	440(20)	-16(19)	-100(20)	-140(20)
C(41)	3280(150)	3250(140)	780(70)	490(80)	-270(80)	-2870(130)
C(42)	1420(80)	620(50)	1390(80)	-40(50)	-600(60)	-310(50)
C(43)	620(40)	1130(60)	510(40)	-290(40)	-70(30)	250(40)
C(44)	660(40)	1410(70)	610(40)	220(40)	10(30)	-220(40)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for IAT21 (CCDC 698486).

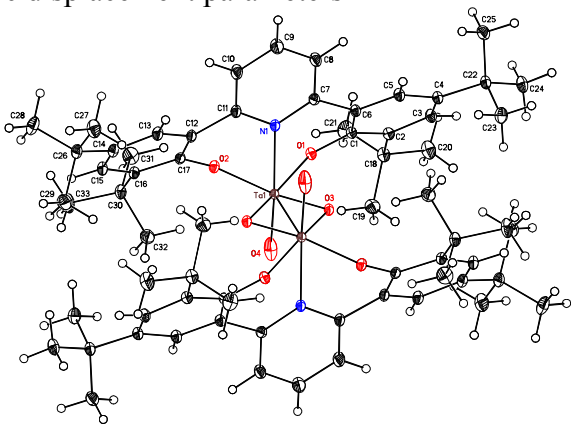
	x	y	z	U_{iso}
H(3)	2862(8)	11210(20)	740(30)	23(11)
H(5)	3480(7)	11150(20)	3440(30)	10(10)
H(8)	3471(8)	10200(20)	4900(30)	19(12)
H(9)	3822(9)	9560(30)	6410(40)	56(15)
H(10)	4091(7)	8300(20)	5870(30)	14(10)
H(13)	4450(8)	8050(30)	4960(30)	24(13)
H(15)	4686(10)	5820(30)	3420(40)	53(15)
H(19A)	2453(9)	9270(30)	1560(40)	47(14)
H(19B)	2635(10)	8220(30)	1510(40)	64(16)
H(19C)	2365(10)	8540(30)	550(30)	48(14)
H(20A)	2405(8)	9720(20)	-870(30)	22(11)
H(20B)	2664(8)	10420(30)	-660(30)	22(13)
H(20C)	2431(9)	10540(30)	120(40)	50(15)
H(21A)	2684(9)	8390(30)	-880(30)	41(13)
H(21B)	3000(9)	8130(30)	20(30)	50(15)
H(21C)	2973(9)	9000(30)	-710(30)	41(15)
H(23A)	3220(9)	12590(30)	520(30)	44(13)
H(23B)	3565(9)	12590(30)	1430(30)	45(13)
H(23C)	3370(8)	13520(30)	1140(30)	33(12)
H(24A)	3338(8)	13560(30)	3150(30)	29(13)
H(24B)	3540(8)	12680(30)	3360(30)	31(12)
H(24C)	3194(9)	12700(30)	3760(30)	46(12)
H(25A)	2895(9)	13550(30)	1860(40)	49(16)
H(25B)	2781(8)	12670(30)	2410(30)	42(13)
H(25C)	2769(9)	12710(30)	1130(40)	48(13)
H(27A)	5155	7157	6450	73
H(27B)	4883	6450	6288	73
H(27C)	4841	7601	6379	73
H(28A)	5332	6711	4836	106
H(28B)	5123	6572	3686	106
H(28C)	5101	5850	4671	106
H(29A)	4874	8697	4926	101
H(29B)	4983	8367	3842	101
H(29C)	5201	8384	4983	101
H(27D)	4858	7908	6194	109
H(27E)	4897	8618	5217	109
H(27F)	5170	8085	5918	109
H(28D)	4998	8006	3479	88
H(28E)	5049	6867	3329	88
H(28F)	5284	7498	4112	88
H(29D)	5256	6320	5664	97
H(29E)	5035	5714	4794	97
H(29F)	4951	6020	5932	97
H(31A)	4030(10)	4280(30)	3310(40)	64(17)
H(31B)	3895(11)	3940(40)	1990(40)	88(19)
H(31C)	3761(11)	4820(30)	2560(40)	68(18)
H(32A)	3850(10)	6130(30)	1080(40)	69(16)
H(32B)	3989(11)	5110(40)	520(40)	83(19)

H(32C)	4215(10)	5980(30)	840(40)	66(18)
H(33A)	4571(12)	5040(40)	1790(50)	90(20)
H(33B)	4366(11)	4130(40)	1570(40)	80(20)
H(33C)	4510(11)	4280(30)	2880(40)	67(18)
H(34A)	3354(10)	6220(30)	540(40)	60(19)
H(34B)	3049(11)	6420(30)	590(40)	73(18)
H(34C)	3207(14)	5640(40)	1310(50)	130(30)
H(35A)	2742(10)	6500(30)	2830(40)	64(16)
H(35B)	2850(8)	7630(30)	3150(30)	45(14)
H(35C)	2842(9)	6780(30)	4100(40)	50(14)
H(36A)	3215(8)	5640(20)	4450(30)	25(12)
H(36B)	3482(8)	5520(20)	3870(30)	29(12)
H(36C)	3108(10)	5300(30)	3370(40)	61(18)
H(41A)	4677	10058	6890	378
H(41B)	4585	11178	6901	378
H(41C)	4379	10411	6176	378
H(42A)	4490	10528	8473	150
H(42B)	4184	10658	7685	150
H(43A)	4029	9408	8697	93
H(43B)	4344	9194	9377	93
H(44A)	4012	7829	7982	136
H(44B)	4058	7800	9284	136
H(44C)	4324	7617	8684	136

Crystal Structure Analysis of:

Complex 7 (IAT06)

Contents



IAT06

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 683409. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 683409."

Table 1. Crystal data and structure refinement for IAT06 (CCDC 683409).

Empirical formula	$C_{66}H_{86}N_2O_8Ta_2 \cdot 4(CH_2Cl_2)$
Formula weight	1736.97
Crystallization Solvent	Petroleum ether
Crystal Habit	Block
Crystal size	0.25 x 0.23 x 0.14 mm^3
Crystal color	Colorless

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9853 reflections used in lattice determination	2.87 to 51.25°
Unit cell dimensions	a = 16.0570(7) Å b = 12.8407(6) Å β= 103.542(3)° c = 18.4561(9) Å
Volume	3699.5(3) $Å^3$
Z	2
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.559 Mg/m^3
F(000)	1748
Data collection program	Bruker APEX2 v2.1-0
θ range for data collection	1.95 to 51.56°
Completeness to θ = 51.56°	98.9 %
Index ranges	$-35 \leq h \leq 28$, $-27 \leq k \leq 28$, $-40 \leq l \leq 40$
Data collection scan type	ω scans; 31 settings
Data reduction program	Bruker SAINT-Plus v7.34A
Reflections collected	331499
Independent reflections	41036 [R_{int}= 0.0418]
Absorption coefficient	3.297 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7501 and 0.6005

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	41036 / 0 / 418
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.629
Final R indices [$I>2\sigma(I)$, 31962 reflections]	R1 = 0.0250, *w*R2 = 0.0388
R indices (all data)	R1 = 0.0440, *w*R2 = 0.0400
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.009
Average shift/error	0.000
Largest diff. peak and hole	3.987 and -2.005 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The identity of the terminal ligand (O4) on Ta is ambiguous. Based on bond distance it appears to be oxygen and therefore an OH group. The location of an hydrogen is notoriously difficult in third row transition metals and it is not included in the model as its position would be arbitrary. One large peak in the difference map is ~1.4Å from O4 and is believed to arise from incomplete absorption correction.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

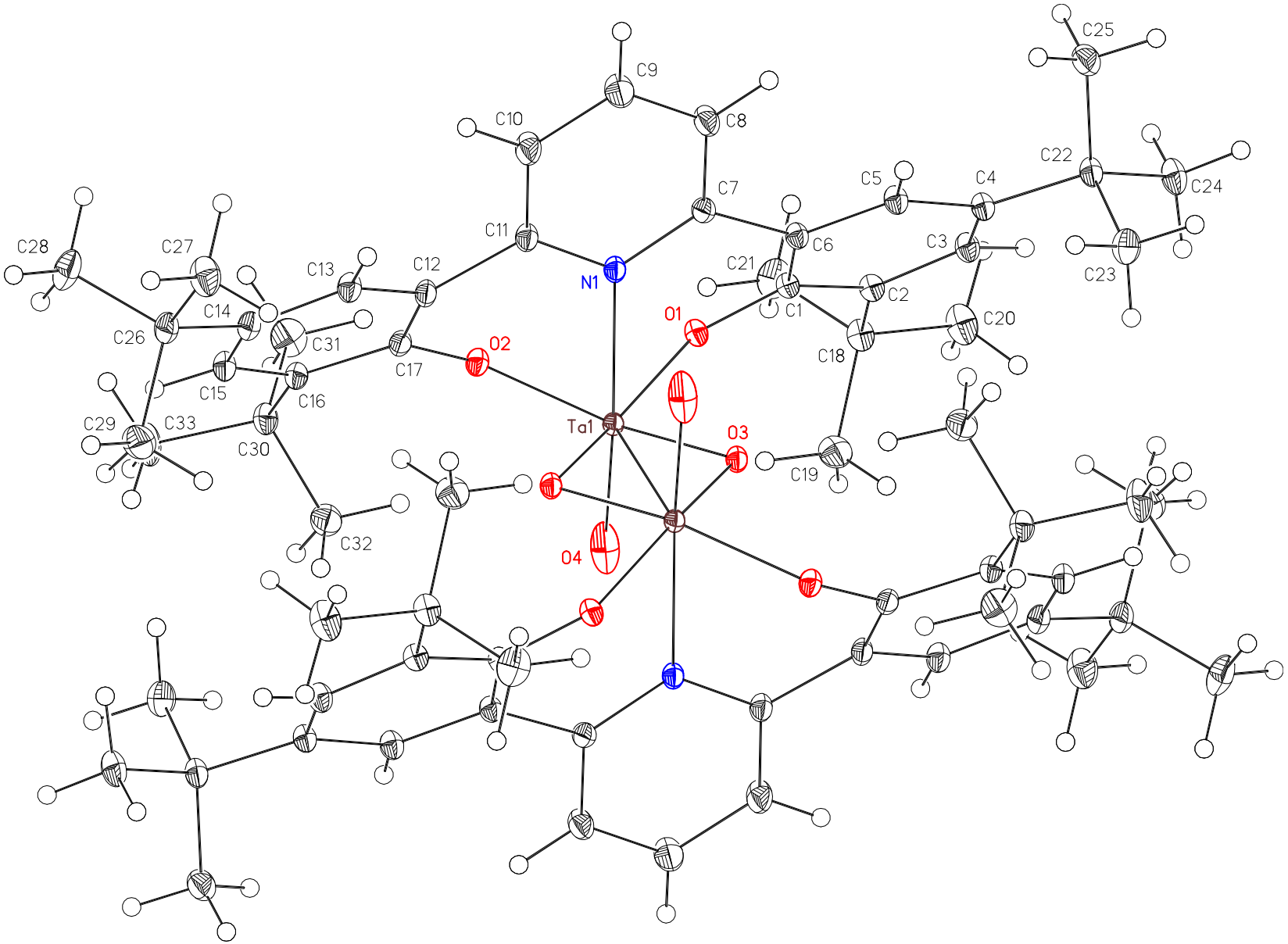

C25
C9
C10
C8
C22
C5
C4
C24
C7
C28
C27
C11
C6
C3
C13
C12
N1
C21
C2
C23
C14
C1
O1
C20
C26
C31
O2
C18
C17
C15
C16
Ta1
O3
C29
C33
C30
C19
C32
O4

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for IAT06 (CCDC 683409). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ta(1)	5209(1)	9163(1)	4507(1)	9(1)
O(1)	4520(1)	7954(1)	4103(1)	11(1)
O(2)	6325(1)	8491(1)	4592(1)	11(1)
O(3)	4236(1)	9768(1)	4801(1)	11(1)
O(4)	5149(1)	9889(1)	3492(1)	26(1)
N(1)	5332(1)	8109(1)	5542(1)	10(1)
C(1)	3814(1)	7596(1)	4307(1)	10(1)
C(2)	3083(1)	7318(1)	3756(1)	11(1)
C(3)	2347(1)	7060(1)	3998(1)	12(1)
C(4)	2304(1)	7075(1)	4742(1)	11(1)
C(5)	3057(1)	7294(1)	5273(1)	12(1)
C(6)	3826(1)	7524(1)	5069(1)	10(1)
C(7)	4640(1)	7565(1)	5653(1)	11(1)
C(8)	4698(1)	6990(1)	6300(1)	16(1)
C(9)	5462(1)	6958(1)	6839(1)	20(1)
C(10)	6168(1)	7472(1)	6706(1)	18(1)
C(11)	6098(1)	8041(1)	6052(1)	12(1)
C(12)	6883(1)	8521(1)	5902(1)	11(1)
C(13)	7558(1)	8799(1)	6510(1)	13(1)
C(14)	8347(1)	9116(1)	6405(1)	13(1)
C(15)	8464(1)	9104(1)	5677(1)	13(1)
C(16)	7822(1)	8854(1)	5052(1)	12(1)
C(17)	7006(1)	8615(1)	5179(1)	11(1)
C(18)	3082(1)	7324(1)	2928(1)	13(1)
C(19)	3236(1)	8435(1)	2677(1)	18(1)
C(20)	2221(1)	6952(1)	2444(1)	19(1)
C(21)	3776(1)	6587(1)	2776(1)	20(1)
C(22)	1462(1)	6883(1)	4978(1)	12(1)
C(23)	1196(1)	7899(1)	5299(1)	17(1)
C(24)	732(1)	6560(1)	4320(1)	17(1)
C(25)	1585(1)	6023(1)	5570(1)	18(1)
C(26)	9074(1)	9498(1)	7046(1)	14(1)
C(27)	8846(1)	9413(1)	7801(1)	21(1)
C(28)	9890(1)	8852(1)	7080(1)	22(1)
C(29)	9256(1)	10642(1)	6902(1)	21(1)
C(30)	7983(1)	8835(1)	4266(1)	14(1)
C(31)	7781(1)	7749(1)	3923(1)	21(1)
C(32)	7426(1)	9650(1)	3763(1)	19(1)
C(33)	8924(1)	9073(1)	4272(1)	22(1)
C(41)	1709(1)	3688(1)	3999(1)	24(1)
Cl(1)	1726(1)	4014(1)	3077(1)	42(1)
Cl(2)	659(1)	3602(1)	4124(1)	29(1)
C(42)	4285(1)	4102(1)	5696(1)	44(1)
Cl(3)	3799(1)	4440(1)	6420(1)	53(1)
Cl(4)	3795(1)	4688(1)	4839(1)	48(1)

Table 3. Selected bond lengths [Å] and angles [°] for IAT06 (CCDC 683409).

Ta(1)-O(3)	1.9328(5)	O(3)-Ta(1)-O(3)#1	78.95(2)
Ta(1)-O(3)#1	1.9431(5)	O(3)-Ta(1)-O(1)	90.25(2)
Ta(1)-O(1)	1.9502(5)	O(3)#1-Ta(1)-O(1)	160.96(2)
Ta(1)-O(2)	1.9623(5)	O(3)-Ta(1)-O(2)	159.60(2)
Ta(1)-O(4)	2.0733(8)	O(3)#1-Ta(1)-O(2)	89.29(2)
Ta(1)-N(1)	2.3119(6)	O(1)-Ta(1)-O(2)	96.07(2)
Ta(1)-Ta(1)#1	2.99175(11)	O(3)-Ta(1)-O(4)	101.76(2)
O(3)-Ta(1)#1	1.9431(5)	O(3)#1-Ta(1)-O(4)	101.13(2)
		O(1)-Ta(1)-O(4)	96.37(2)
		O(2)-Ta(1)-O(4)	96.80(2)
		O(3)-Ta(1)-N(1)	85.50(2)
		O(3)#1-Ta(1)-N(1)	86.16(2)
		O(1)-Ta(1)-N(1)	77.32(2)
		O(2)-Ta(1)-N(1)	77.05(2)
		O(4)-Ta(1)-N(1)	170.51(2)
		O(3)-Ta(1)-Ta(1)#1	39.603(14)
		O(3)#1-Ta(1)-Ta(1)#1	39.348(14)
		O(1)-Ta(1)-Ta(1)#1	128.080(15)
		O(2)-Ta(1)-Ta(1)#1	126.687(15)
		O(4)-Ta(1)-Ta(1)#1	104.896(19)
		N(1)-Ta(1)-Ta(1)#1	84.590(15)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1

Table 4. Bond lengths [Å] and angles [°] for IAT06 (CCDC 683409).

Ta(1)-O(3)	1.9328(5)	O(3)-Ta(1)-O(3)#1	78.95(2)
Ta(1)-O(3)#1	1.9431(5)	O(3)-Ta(1)-O(1)	90.25(2)
Ta(1)-O(1)	1.9502(5)	O(3)#1-Ta(1)-O(1)	160.96(2)
Ta(1)-O(2)	1.9623(5)	O(3)-Ta(1)-O(2)	159.60(2)
Ta(1)-O(4)	2.0733(8)	O(3)#1-Ta(1)-O(2)	89.29(2)
Ta(1)-N(1)	2.3119(6)	O(1)-Ta(1)-O(2)	96.07(2)
Ta(1)-Ta(1)#1	2.99175(11)	O(3)-Ta(1)-O(4)	101.76(2)
O(1)-C(1)	1.3552(8)	O(3)#1-Ta(1)-O(4)	101.13(2)
O(2)-C(17)	1.3569(8)	O(1)-Ta(1)-O(4)	96.37(2)
O(3)-Ta(1)#1	1.9431(5)	O(2)-Ta(1)-O(4)	96.80(2)
N(1)-C(11)	1.3652(8)	O(3)-Ta(1)-N(1)	85.50(2)
N(1)-C(7)	1.3677(9)	O(3)#1-Ta(1)-N(1)	86.16(2)
C(1)-C(6)	1.4050(10)	O(1)-Ta(1)-N(1)	77.32(2)
C(1)-C(2)	1.4074(9)	O(2)-Ta(1)-N(1)	77.05(2)
C(2)-C(3)	1.3970(10)	O(4)-Ta(1)-N(1)	170.51(2)
C(2)-C(18)	1.5283(10)	O(3)-Ta(1)-Ta(1)#1	39.603(14)
C(3)-C(4)	1.3926(10)	O(3)#1-Ta(1)-Ta(1)#1	39.348(14)
C(4)-C(5)	1.3948(9)	O(1)-Ta(1)-Ta(1)#1	128.080(15)
C(4)-C(22)	1.5336(10)	O(2)-Ta(1)-Ta(1)#1	126.687(15)
C(5)-C(6)	1.4032(9)	O(4)-Ta(1)-Ta(1)#1	104.896(19)
C(6)-C(7)	1.4882(8)	N(1)-Ta(1)-Ta(1)#1	84.590(15)
C(7)-C(8)	1.3890(10)	C(1)-O(1)-Ta(1)	126.89(4)
C(8)-C(9)	1.3867(10)	C(17)-O(2)-Ta(1)	124.29(4)
C(9)-C(10)	1.3829(11)	Ta(1)-O(3)-Ta(1)#1	101.05(2)
C(10)-C(11)	1.3926(10)	C(11)-N(1)-C(7)	119.74(6)
C(11)-C(12)	1.4873(9)	C(11)-N(1)-Ta(1)	119.75(4)
C(12)-C(17)	1.3978(10)	C(7)-N(1)-Ta(1)	120.50(4)
C(12)-C(13)	1.4108(9)	O(1)-C(1)-C(6)	118.95(5)
C(13)-C(14)	1.3864(10)	O(1)-C(1)-C(2)	119.73(6)
C(14)-C(15)	1.4004(11)	C(6)-C(1)-C(2)	121.31(6)
C(14)-C(26)	1.5346(9)	C(3)-C(2)-C(1)	117.03(6)
C(15)-C(16)	1.3936(10)	C(3)-C(2)-C(18)	121.20(6)
C(16)-C(17)	1.4174(9)	C(1)-C(2)-C(18)	121.74(6)
C(16)-C(30)	1.5307(11)	C(4)-C(3)-C(2)	123.56(6)
C(18)-C(20)	1.5366(10)	C(3)-C(4)-C(5)	117.41(6)
C(18)-C(19)	1.5364(11)	C(3)-C(4)-C(22)	121.91(6)
C(18)-C(21)	1.5375(11)	C(5)-C(4)-C(22)	120.67(6)
C(22)-C(25)	1.5331(11)	C(4)-C(5)-C(6)	121.78(7)
C(22)-C(24)	1.5346(10)	C(5)-C(6)-C(1)	118.43(6)
C(22)-C(23)	1.5352(11)	C(5)-C(6)-C(7)	119.43(6)
C(26)-C(27)	1.5262(12)	C(1)-C(6)-C(7)	121.76(6)
C(26)-C(29)	1.5339(11)	N(1)-C(7)-C(8)	120.48(6)
C(26)-C(28)	1.5405(10)	N(1)-C(7)-C(6)	121.06(6)
C(30)-C(31)	1.5341(11)	C(8)-C(7)-C(6)	118.37(6)
C(30)-C(33)	1.5377(10)	C(9)-C(8)-C(7)	120.12(7)
C(30)-C(32)	1.5402(11)	C(10)-C(9)-C(8)	118.94(7)
C(41)-Cl(1)	1.7584(11)	C(9)-C(10)-C(11)	119.99(6)
C(41)-Cl(2)	1.7586(9)	N(1)-C(11)-C(10)	120.59(6)
C(42)-Cl(3)	1.7518(16)	N(1)-C(11)-C(12)	120.74(6)
C(42)-Cl(4)	1.7622(15)	C(10)-C(11)-C(12)	118.58(6)
		C(17)-C(12)-C(13)	118.88(6)

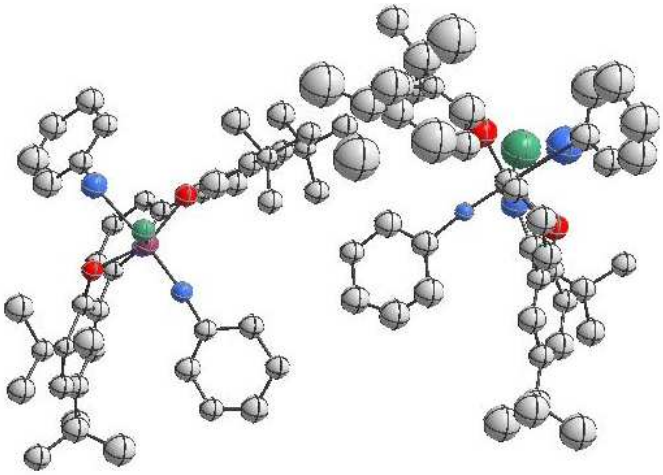
C(17)-C(12)-C(11)	121.96(6)	C(25)-C(22)-C(24)	108.47(6)
C(13)-C(12)-C(11)	118.89(7)	C(4)-C(22)-C(24)	112.28(6)
C(14)-C(13)-C(12)	121.32(7)	C(25)-C(22)-C(23)	109.79(7)
C(13)-C(14)-C(15)	117.62(6)	C(4)-C(22)-C(23)	108.44(6)
C(13)-C(14)-C(26)	122.78(7)	C(24)-C(22)-C(23)	107.71(6)
C(15)-C(14)-C(26)	119.57(6)	C(27)-C(26)-C(29)	108.80(7)
C(16)-C(15)-C(14)	123.84(6)	C(27)-C(26)-C(14)	112.32(6)
C(15)-C(16)-C(17)	116.48(7)	C(29)-C(26)-C(14)	108.35(6)
C(15)-C(16)-C(30)	122.05(6)	C(27)-C(26)-C(28)	107.95(7)
C(17)-C(16)-C(30)	121.47(6)	C(29)-C(26)-C(28)	109.12(7)
O(2)-C(17)-C(12)	118.91(6)	C(14)-C(26)-C(28)	110.26(6)
O(2)-C(17)-C(16)	119.76(6)	C(16)-C(30)-C(31)	109.82(7)
C(12)-C(17)-C(16)	121.32(6)	C(16)-C(30)-C(33)	111.97(6)
C(2)-C(18)-C(20)	111.64(6)	C(31)-C(30)-C(33)	107.25(6)
C(2)-C(18)-C(19)	110.11(6)	C(16)-C(30)-C(32)	110.92(6)
C(20)-C(18)-C(19)	107.45(6)	C(31)-C(30)-C(32)	109.36(7)
C(2)-C(18)-C(21)	110.39(6)	C(33)-C(30)-C(32)	107.42(7)
C(20)-C(18)-C(21)	107.11(6)	Cl(1)-C(41)-Cl(2)	111.97(5)
C(19)-C(18)-C(21)	110.05(7)	Cl(3)-C(42)-Cl(4)	113.18(6)
C(25)-C(22)-C(4)	110.10(6)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1

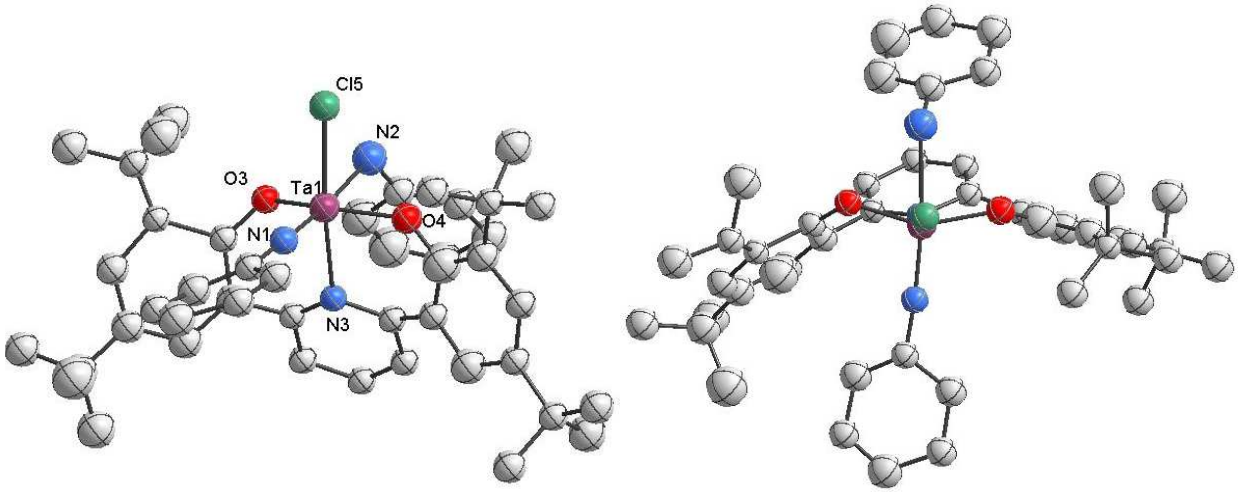
Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for IAT06 (CCDC 683409). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ta(1)	72(1)	98(1)	92(1)	11(1)	14(1)	-1(1)
O(1)	95(2)	129(2)	103(2)	-2(2)	30(2)	-16(1)
O(2)	86(2)	138(2)	101(2)	0(2)	12(2)	3(1)
O(3)	76(2)	112(2)	124(2)	-4(2)	16(2)	-4(1)
O(4)	145(2)	358(4)	291(4)	-165(3)	66(2)	-41(2)
N(1)	77(2)	122(2)	104(2)	3(2)	16(2)	-4(2)
C(1)	95(2)	110(2)	98(2)	-5(2)	27(2)	-8(2)
C(2)	109(2)	127(2)	94(2)	-10(2)	23(2)	-10(2)
C(3)	102(2)	153(3)	105(3)	-12(2)	14(2)	-20(2)
C(4)	94(2)	135(2)	112(3)	-4(2)	23(2)	-14(2)
C(5)	99(2)	154(3)	98(2)	-2(2)	22(2)	-15(2)
C(6)	90(2)	122(2)	96(2)	-3(2)	16(2)	-12(2)
C(7)	97(2)	122(2)	113(2)	14(2)	6(2)	-8(2)
C(8)	115(2)	218(3)	135(3)	51(2)	21(2)	-27(2)
C(9)	145(3)	293(4)	150(3)	95(3)	10(3)	-25(3)
C(10)	110(2)	264(3)	144(3)	70(3)	-4(2)	-14(2)
C(11)	85(2)	151(3)	109(3)	8(2)	14(2)	0(2)
C(12)	76(2)	137(2)	120(3)	7(2)	16(2)	4(2)
C(13)	97(2)	163(3)	117(3)	1(2)	14(2)	0(2)
C(14)	89(2)	146(2)	134(3)	-3(2)	8(2)	5(2)
C(15)	88(2)	159(3)	148(3)	-1(2)	23(2)	-3(2)
C(16)	92(2)	126(2)	134(3)	0(2)	34(2)	7(2)
C(17)	84(2)	113(2)	118(3)	0(2)	17(2)	9(2)
C(18)	129(2)	175(3)	96(3)	-23(2)	29(2)	-17(2)
C(19)	192(3)	218(3)	120(3)	29(2)	26(2)	-19(2)
C(20)	172(3)	286(4)	114(3)	-46(3)	15(2)	-58(3)
C(21)	202(3)	244(4)	165(3)	-58(3)	62(3)	27(3)
C(22)	91(2)	164(3)	114(3)	3(2)	22(2)	-16(2)
C(23)	140(3)	209(3)	163(3)	-26(2)	42(2)	3(2)
C(24)	112(2)	230(3)	151(3)	-20(2)	17(2)	-42(2)
C(25)	142(3)	220(3)	179(3)	56(2)	38(3)	-24(2)
C(26)	97(2)	170(3)	145(3)	-6(2)	-3(2)	-7(2)
C(27)	158(3)	303(4)	143(3)	-11(3)	-1(3)	-37(3)
C(28)	125(3)	261(4)	236(4)	-34(3)	-20(3)	43(2)
C(29)	190(3)	184(3)	225(4)	-16(3)	8(3)	-43(2)
C(30)	108(2)	174(3)	142(3)	-6(2)	48(2)	1(2)
C(31)	235(3)	206(3)	225(4)	-67(3)	99(3)	0(3)
C(32)	172(3)	228(3)	172(3)	57(3)	55(3)	2(2)
C(33)	122(3)	345(4)	198(4)	-13(3)	77(3)	-20(3)
C(41)	176(3)	275(4)	267(4)	26(3)	66(3)	52(3)
Cl(1)	401(1)	500(2)	413(2)	251(1)	216(1)	170(1)
Cl(2)	224(1)	244(1)	433(2)	12(1)	160(1)	8(1)
C(42)	340(5)	329(6)	641(9)	15(6)	79(6)	148(4)
Cl(3)	558(2)	248(1)	861(3)	-85(2)	338(2)	-111(1)
Cl(4)	275(1)	391(2)	690(2)	32(2)	-73(1)	1(1)

Structure Drawings of Complex 5



The crystal is twinned; one of the two molecules in the asymmetric unit (right) prevents proper refinement of the system.



Despite the lack of refinement, the C_s-symmetry of the *bis*(phenolate)pyridine ligand is apparent.